Applying no-depletion equilibrium sampling and full-depletion bioaccessibility extraction to 35 historically polycyclic aromatic hydrocarbon contaminated soils

Assessing the bioaccessibility of organic pollutants in contaminated soils is considered a complement to measurements of total concentrations in risk assessment and legislation. Consequently, methods for its quantification require validation with historically contaminated soils. In this study, 35 such soils were obtained from various locations in Switzerland and Cuba. They were exposed to different pollution sources (e.g., pyrogenic and petrogenic) at various distances (i.e., urban to rural) and were subject to different land use (e.g., urban gardening and forest). Passive equilibrium sampling with polyoxymethylene was used to determine freely dissolved concentrations \( C_{\text{free}} \) of polycyclic aromatic hydrocarbons (PAHs), while sorptive bioaccessibility extraction (SBE) with silicone rods was used to determine the bioaccessible PAH concentrations \( C_{\text{bioacc}} \) of these soils. The organic carbon partition coefficients of the soils were highest for skeet soils, followed by traffic, urban garden and rural soils. Lowest values were obtained from soil exposed to petrogenic sources. Applicability of SBE to quantify \( C_{\text{bioacc}} \) was restricted by silicone rod sorption capacity, as expressed quantitatively by the Sorption Capacity Ratio (SCR); particularly for soils with very high \( K_D \). The source of contamination determined bioaccessible fractions \( f_{\text{bioacc}} \). The smallest \( f_{\text{bioacc}} \) were obtained with skeet soils (15%), followed by the pyrogenically influenced soils, rural soils, and finally, the petrogenically contaminated soil (71%). In conclusion, we present the potential and limitations of the SBE method to quantify bioaccessibility in real soils. These results can be used for additional development of this and similar bioaccessibility methods to guarantee sufficient sorption capacity to obtain reliable results. Freely dissolved concentrations and bioaccessible fractions of PAHs in soils depended on pollutant source and site characteristics, while the sink capacity was limiting during bioaccessibility extractions of soils with low PAH content and high \( K_D \) values.

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Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Agroscope, Swiss Federal Institute of Technology Zurich, Universidad de La Habana
Contributors: Bartolomè, N., Hilber, I., Sosa, D., Schulin, R., Mayer, P., Bucheli, T. D.
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Determining Biodegradation Kinetics of Hydrocarbons at Low Concentrations: Covering 5 and 9 Orders of Magnitude of Kow and Kaw

A partitioning-based experimental platform was developed and applied to determine primary biodegradation kinetics of 53 hydrocarbons at ng/L to μg/L concentrations covering C8-C20, 11 structural classes, and several orders of magnitude in hydrophobicity and volatility: (1) Passive dosing from a loaded silicone donor was used to set the concentration of each hydrocarbon in mixture stock solutions; (2) these solutions were combined with environmental water samples in gastight auto sampler vials for 1-100 days incubation, and (3) automated solid phase microextraction (SPME) coupled to GC-MS was applied directly on these test systems for measuring primary biodegradation relative to abiotic controls. First order biodegradation kinetics were obtained for 40 hydrocarbons in activated sludge filtrate, 18 in seawater, and 21 in lake water. Water phase half-lives in seawater and lake water were poorly related to hydrophobicity and volatility but were, with a few exceptions, within a factor of 10 or shorter than BioHCwin predictions. The most persistent hydrocarbons, 1,1,4,4,6-pentamethyldecaline, perhydroyrene, 1,2,3,6,7,8-hexahydropyrene, and 2,2,4,4,6,8,8-heptamethylnonane, showed limited or inconsistent degradation in all three environmental media. This biodegradation approach can cover a large chemical space at low substrate concentrations, which makes it highly suited for optimizing predictive models for environmental biodegradation.
A Chemical Activity Approach to Exposure and Risk Assessment of Chemicals

To support the goals articulated in the vision for exposure and risk assessment in the twenty-first century, we highlight the application of a thermodynamic chemical activity approach for the exposure and risk assessment of chemicals in the environment. The present article describes the chemical activity approach, its strengths and limitations, and provides examples of how this concept may be applied to the management of single chemicals and chemical mixtures. The examples demonstrate that the chemical activity approach provides a useful framework for 1) compiling and evaluating exposure and toxicity information obtained from many different sources, 2) expressing the toxicity of single and multiple chemicals, 3) conducting hazard and risk assessments of single and multiple chemicals, 4) identifying environmental exposure pathways, and 5) reducing error and characterizing uncertainty in risk assessment. The article further illustrates that the chemical activity approach can support an adaptive management strategy for environmental stewardship of chemicals where “safe” chemical activities are established based on toxicological studies and presented as guidelines for environmental quality in various environmental media that can be monitored by passive sampling and other techniques.

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Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Simon Fraser University, ExxonMobil, United States Environmental Protection Agency, TG Environmental Research, Radboud University Nijmegen
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Scopus rating (2015): CiteScore 3 SJR 1.433 SNIP 1.056
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Scopus rating (2013): CiteScore 2.88 SJR 1.656 SNIP 1.086
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): CiteScore 2.81 SJR 1.639 SNIP 1.108
Assessing PCB pollution in the Baltic Sea - An equilibrium partitioning based study

Sediment cores and bottom water samples from across the Baltic Sea region were analyzed for freely dissolved concentrations (C_{free}), total sediment concentrations (CT) and the dissolved aqueous fraction in water of seven indicator PCBs. Ex-situ equilibrium sampling of sediment samples was conducted with polydimethylsiloxane (PDMS) coated glass fibers that were analyzed by automated thermal desorption GC-MS, which yielded PCB concentrations in the fiber coating (CPDMS). Measurements of CPDMS and CT were then applied to determine (i) spatially resolved freely dissolved PCB concentrations; (ii) baseline toxicity potential based on chemical activities (a); (iii) site specific mixture compositions; (iv) diffusion gradients at the sediment water interface and within the sediment cores; and (vi) site specific distribution ratios (KD). The contamination levels were low in the Gulf of Finland and moderate to elevated in the Baltic Proper, with the highest levels observed in the western Baltic Sea. The SPME method has been demonstrated to be an appropriate and sensitive tool for area surveys presenting new opportunities to study the in-situ distribution and thermodynamics of hydrophobic organic chemicals at trace levels in marine environments.
Equilibrium sampling reveals increasing thermodynamic potential of polycyclic aromatic hydrocarbons during sewage sludge digestion

The reuse of digested sludge from wastewater treatment plants (WWTPs) as soil fertilizer poses a risk for contamination of soil and water environments. The present study provides a new approach for investigating the exposure of hydrophobic organic chemicals in sewage sludge. The methodology of equilibrium sampling with multiple thicknesses of silicone was successfully validated and applied to complex sludge matrices. Polycyclic aromatic hydrocarbon (PAH) concentrations in silicone (Csilicone) were determined and compared across four WWTPs. Activity ratios (ARs), defined as Csilicone at equilibrium with digested sludge (final product) over Csilicone at equilibrium with secondary sludge (intermediate product), were in the range 0.85-20 with all except one AR>1. These ARs thus revealed increased thermodynamic potential of both parent and alkylated PAHs in digested sludge compared with secondary sludge, and thereby higher exposure of PAHs in sludge after digestion than before digestion. This observation can be explained by the concept of "solvent depletion" as organic matter decreased by a factor of 1.3 during digestion, resulting in reduced sorptive capacity and increased freely dissolved concentrations (Cfree). The PAHs with logKow > 6 had ARs close to 1.3, whereas PAHs with logKow <6 showed higher ARs than the organic matter decrease factor of 1.3. Cfree in digested sludge were higher than reported in rural soil and generally consistent with levels reported for Baltic Sea sediment.

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Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, Technical University of Denmark, Helmholtz Center for Environmental Research (UFZ), University of Copenhagen
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Headspace passive dosing of volatile hydrophobic chemicals – Aquatic toxicity testing exactly at the saturation level

It is challenging to conduct aquatic tests with highly hydrophobic and volatile chemicals while avoiding substantial sorptive and evaporative losses. A simple and versatile headspace passive dosing (HS-PD) method was thus developed for such chemicals: The pure liquid test chemical was added to a glass insert, which was then placed with the open end in the headspace of a closed test system containing aqueous test medium. The test chemical served as the dominating partitioning donor for establishing and maintaining maximum exposure levels in the headspace and aqueous solution, without direct contact between the donor and the test medium. The HS-PD method was cross validated against passive dosing with a saturated silicone elastomer, using headspace gas chromatography as analytical instrument and saturated vapors as reference. The HS-PD method was then applied to control the exposure in algal growth inhibition tests with the green algae Raphidocelis subcapitata. The model chemicals were C9-C14 n-alkanes and the cyclic volatile methyl siloxanes octamethyltetraacyclosiloxane (D4) and decamethylpentacyclosiloxane (D5). Growth rate inhibition at the solubility limit was 100% for C9-C13 n-alkanes and 53±31% (95% CI) for tetradecane. A moderate inhibition of 11±4% (95% CI) was observed for D4, whereas no inhibition was observed for D5. The present study introduces an effective method for aquatic toxicity testing of a difficult-to-test group of chemicals and provides an improved experimental basis for investigating toxicity cut-offs.
Linking algal growth inhibition to chemical activity: Excess toxicity below 0.1% of saturation

Chemical activity quantifies the energetic level of an organic compound relative to its pure liquid [0–1], and several studies have reported that baseline toxicity generally requires chemical activities of 0.01–0.1. The first aim was to challenge this chemical activity range for baseline toxicity. Algal growth inhibition data (median effective concentrations, EC_{50}) were compiled from two recent studies and included 108 compounds categorised as non-polar (mode of action, MOA1) and polar (MOA2) narcotics. These data were linked to chemical activity by (1) plotting them relative to a regression for
(subcooled) liquid solubility (SL), which served as visual reference for chemical activity of unity and (2) determining EC\textsubscript{50}/SL ratios that essentially equal median effective chemical activity (Ea\textsubscript{50}). Growth inhibition required chemical activity >0.01 for MOA1 and >0.001 for MOA2 compounds. The second aim was to identify compounds exerting excess toxicity, i.e., when growth inhibition occurred at chemical activity <0.001. From a recent review with 2323 data entries, 315 EC\textsubscript{50} values passed our selection criteria. 280 of these EC\textsubscript{50} values were within or near the baseline toxicity range (Ea\textsubscript{50} >0.001), and 25 compounds were found to exert excess toxicity (Ea\textsubscript{50} <0.001). Of these compounds, 16 are pesticides or precursors. Methodologically, this study includes two methods for translating EC\textsubscript{50} values into the chemical activity framework, each having advantages and limitations. Scientifically, this study confirms that baseline toxicity generally requires chemical activities of 0.01–0.1 and extends the application of the chemical activity approach beyond baseline toxicity, by demonstrating its utility to identify compounds that exert excess toxicity.

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Organisations: Department of Environmental Engineering, Environmental Fate & Effect of Chemicals, ARC Arnot Research & Consulting Inc., Trent University
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Web of Science (2014): Impact factor 3.34
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Meta-Analysis of Fish Early Life Stage Tests - Association of Toxic Ratios and Acute-To-Chronic Ratios with Modes of Action

Fish early life stage (FELS) tests (OECD test guideline 210) are widely conducted to estimate chronic fish toxicity. In these tests, fish are exposed from the embryonic to the juvenile life stage. In order to analyse whether certain modes of action are related to high toxic ratios (TR, i.e., ratios between experimental effect and baseline toxicity) and/or acute-to-chronic ratios (ACR) in the FELS test effect concentrations for 183 compounds were extracted from the US EPA ecotoxicity database. Analysis of effect concentration of narcotic compounds indicated that baseline toxicity could be observed in the FELS test at similar concentrations as in acute fish toxicity test. All non-narcotic modes of action were associated with higher TRs with median values ranging from 4 to 9.3*10^4 (uncoupling<reactivity<neuromuscular toxicity<hemoglobin formation<endocrine disruption<extracellular matrix formation inhibition). Four modes of action (were also found to be associated with high ACRs: (1) lysyl oxidase inhibition leading to notochord distortion, (2) putative methemoglobin formation or haemolytic anemia, (3) endocrine disruption, and (4) compounds with neuromuscular toxicity. It was discussed that for the prediction of effect concentrations in the FELS test with alternative test systems, endpoints targeted to the modes of action of compounds with enhanced TR or ACR could be used to trigger FELS tests or even replace these tests.

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New approaches for determining solubility of organic chemicals

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Contributors: Birch, H., Trac, N. L., Mayer, P.
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Aquatic toxicity testing of liquid hydrophobic chemicals – Passive dosing exactly at the saturation limit
The aims of the present study were (1) to develop a passive dosing approach for aquatic toxicity testing of liquid substances with very high Kow values and (2) to apply this approach to the model substance dodecylbenzene (DDB, Log Kow = 8.65). The first step was to design a new passive dosing format for testing DDB exactly at its saturation limit. Silicone O-rings were saturated by direct immersion in pure liquid DDB, which resulted in swelling of >14%. These saturated O-rings were used to establish and maintain DDB exposure exactly at the saturation limit throughout 72-h algal growth inhibition tests with green algae Raphidocelis subcapitata. Growth rate inhibition at DDB solubility was 13 ± 5% (95% CI) in a first and 8 ± 3% (95% CI) in a repeated test, which demonstrated that improved exposure control can lead to good precision and repeatability of toxicity tests. This moderate toxicity at chemical activity of unity was higher than expected relative to a reported hydrophobicity cut-off in toxicity, but lower than expected relative to a reported chemical activity range for baseline toxicity. The present study introduces a new effective approach for toxicity testing of an important group of challenging chemicals, while providing a basis for investigating toxicity cut-off theories.

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Organisations: Department of Environmental Engineering, Environmental Chemistry, RWTH Aachen University, Technical University of Denmark
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Bioavailability and bioaccessibility of polycyclic aromatic hydrocarbons from (post-pyrolytically treated) biochars

Bioaccessibility data of PAHs from biochar produced under real world conditions is scarce and the influence of feedstock and various post-pyrolysis treatments common in agriculture, such as co-composting or lacto-fermentation to produce silage fodder, on their bioavailability and bioaccessibility has hardly been studied. The total (C_{total}), and freely dissolved (i.e., bioavailable) concentrations (C_{free}) of the sum of 16 US EPA PAHs of 43 biochar samples produced and treated in such ways ranged from 0.4 to almost 2000 mg/kg, and from 12 to 81 ng/L, respectively, which resulted in very high biochar-water partition coefficients (4.2 ≤ log KD ≤ 8.8 L/kg) for individual PAHs. Thirty three samples were incubated in contaminant traps that combined a diffusive carrier and a sorptive sink. Incubations yielded samples only containing desorption-resistant PAHs (C_{res}). The desorption resistant PAH fraction was dominant, since only eight out of 33 biochar samples showed statistically significant bioaccessible fractions (f_{bioaccessible} = 1 - C_{res}/C_{total}). Bioavailability correlated positively with C_{total}/surface area. Other relationships of bioavailability and -accessibility with the investigated post-pyrolysis processes or elemental composition could not be found. PAH exposure was very limited (low C_{free}, high C_{res}) for all samples with low to moderate C_{total}, whereas higher exposure was determined in some biochars with C_{total} > 10 mg/kg.

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Organisations: Department of Environmental Engineering, Environmental Chemistry, Agroscope, Aarhus University, Norwegian Geotechnical Institute, Ithaka Institute for Carbon Strategies
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Scopus rating (2009): SJR 1.842 SNIP 1.572
Web of Science (2009): Indexed yes
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Scopus rating (2003): SJR 1.321 SNIP 1.323
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Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.924 SNIP 0.978
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Biodegradation of hydrocarbon mixtures in surface waters at environmentally relevant levels - Effect of inoculum origin on kinetics and sequence of degradation

Biodegradation is a dominant removal process for many organic pollutants, and biodegradation tests serve as tools for assessing their environmental fate within regulatory risk assessment. In simulation tests, the inoculum is not standardized, varying in microbial quantity and quality, thereby potentially impacting the observed biodegradation kinetics. In this study we investigated the effect of inoculum origin on the biodegradation kinetics of hydrocarbons for five inocula from surface waters varying in urbanization and thus expected pre-exposure to petroleum hydrocarbons. A new biodegradation method for testing mixtures of hydrophobic chemicals at trace concentrations was demonstrated: Aqueous solutions containing 9 hydrocarbons were generated by passive dosing and diluted with surface water resulting in test systems containing native microorganisms exposed to test substances at ng-μg/L levels. Automated Headspace Solid Phase Microextraction coupled to GC-MS was applied directly to these test systems to determine substrate depletion relative to abiotic controls. Lag phases were generally less than 8 days. First order rate constants were within one order of magnitude for each hydrocarbon in four of the five waters but lower in water from a rural lake. The sequence of degradation between the 9 hydrocarbons showed similar patterns in the five waters indicating the potential for using selected hydrocarbons for benchmarking between biodegradation tests. Degradation half-times were shorter than or within one order of magnitude of BioHCwin predictions for 8 of 9 hydrocarbons. These results showed that location choice is important for biodegradation kinetics and can provide a relevant input to aquatic exposure and fate models.

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Biodegradation testing of chemicals with high Henry’s constants – separating mass and effective concentration reveals higher rate constants

During simulation-type biodegradation tests, volatile chemicals will continuously partition between water phase and headspace. This study addressed how (1) this partitioning affects biodegradation test results and (2) it can be accounted for by combining mass balance and dynamic biodegradation models. An aqueous mixture of 9 (semi)volatile chemicals was first prepared using passive dosing and then diluted with environmental surface water to produce test systems containing concentrations in the ng/L to µg/L range. After incubation for 2 hours to 4 weeks, automated Headspace Solid Phase Microextraction (HS-SPME) was applied directly on the test systems to measure substrate depletion by biodegradation relative to abiotic controls. HS-SPME was also applied to determine air to water partitioning ratios. Water phase biodegradation rate constants, kwater, were up to 72 times higher than test system biodegradation rate constants, ksystem. True water phase degradation rate constants facilitate extrapolation to other air-water systems and are more suitable input parameters for aquatic exposure and fate models. As such, they should be considered more appropriate for
Biodegradation testing of chemicals with high Henry's constants – Separating mass and effective concentration reveals higher rate constants

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risk assessments than test system rate constants.
Biodegradation testing of hydrophobic chemicals in mixtures at low concentrations – covering the chemical space of petroleum hydrocarbons

Petroleum products are complex mixtures of varying composition containing thousands of hydrocarbons each with their own physicochemical properties and degradation kinetics. One approach for risk assessment of these products is therefore to group the hydrocarbons by carbon number and chemical class i.e. hydrocarbon blocks. However, the biodegradation kinetic data varies in quantity and quality for the different hydrocarbon blocks, hampering the characterization of their fate properties. In this study, biodegradation kinetics of a large number of hydrocarbons aiming to cover the chemical space of petroleum hydrocarbons, were therefore determined at ng/L to µg/L concentrations in surface water, seawater and activated sludge filtrate. Two hydrocarbon mixtures were prepared, comprising a total of 53 chemicals including paraffins, naphthenics and aromatic hydrocarbons from C8 to C20. Passive dosing from silicone rod loaded with the mixtures was used to prepare stock solutions. Test systems were then prepared using stock solution diluted with the surface water, seawater or activated sludge filtrate. Test systems were incubated at 20 °C on a roller for up to 98 days and analyzed using GC-MS and fully automated Solid Phase Micro Extraction. Results were normalized to
parallel measurements of abiotic controls prior to evaluation of biodegradation kinetics. Degradation was generally faster in the activated sludge filtrate than in the seawater and lakewater. In the activated sludge filtrate lag phases were < 9 days for the 49 hydrocarbons that were degraded within test duration. Degradation rate constants and corresponding half-lives were determined for 44 of the hydrocarbons. In lakewater and seawater, less test chemicals were degraded within the test duration compared to the activated sludge filtrate.

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Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Web of Science (2015): Impact factor 5.393
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
Cross validation of two partitioning-based sampling approaches in mesocosms containing PCB contaminated field sediment, biota, and activated carbon amendment

The Gold Standard for determining freely dissolved concentrations (Cfree) of hydrophobic organic compounds in sediment interstitial water would be in situ deployment combined with equilibrium sampling, which is generally difficult to achieve. In the present study, ex situ equilibrium sampling with multiple thicknesses of silicone and in situ pre-equilibrium sampling with low density polyethylene (LDPE) loaded with performance reference compounds were applied independently to measure polychlorinated biphenyls (PCBs) in mesocosms with (1) New Bedford Harbor sediment (MA, USA), (2) sediment and biota, and (3) activated carbon amended sediment and biota. The aim was to cross validate the two different sampling approaches. Around 100 PCB congeners were quantified in the two sampling polymers, and the results confirmed the good precision of both methods and were in overall good agreement with recently published silicone to LDPE partition ratios. Further, the methods yielded Cfree in good agreement for all three experiments. The average ratio between Cfree
determined by the two methods was factor 1.4±0.3 (range: 0.6-2.0), and the results thus cross-validated the two sampling approaches. For future investigations, specific aims and requirements in terms of application, data treatment, and data quality requirements should dictate the selection of the most appropriate partitioning-based sampling approach.

**General information**

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- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
- Web of Science (2016): Impact factor 6.198
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
- Web of Science (2015): Impact factor 5.393
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
- Web of Science (2014): Impact factor 5.33
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
- Web of Science (2013): Impact factor 5.481
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
- Web of Science (2012): Impact factor 5.257
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945
- Web of Science (2011): Impact factor 5.228
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 2.979 SNIP 1.726
Determining lower threshold concentrations for synergistic effects

Though only occurring rarely, synergistic interactions between chemicals in mixtures have long been a point of focus. Most studies analyzing synergistic interactions used unrealistically high chemical concentrations. The aim of the present study is to determine the threshold concentration below which proven synergists cease to act as synergists towards the aquatic crustacean Daphnia magna. To do this, we compared several approaches and test-setups to evaluate which approach gives the most conservative estimate for the lower threshold for synergy for three known azole synergists. We focus on synergistic interactions between the pyrethroid insecticide, alpha-cypermethrin, and one of the three azole fungicides prochloraz, propiconazole or epoxiconazole measured on Daphnia magna immobilization. Three different experimental setups were applied: A standard 48h acute toxicity test, an adapted 48h test using passive dosing for constant chemical exposure concentrations, and a 14-day test. Synergy was defined as occurring in mixtures where either EC50 values decreased more than two-fold below what was predicted by concentration addition (horizontal assessment) or as mixtures where the fraction of immobile organisms increased more than two-fold above what was predicted by independent action (vertical assessment). All three tests confirmed the hypothesis of the existence of a lower azole threshold concentration below which no synergistic interaction was observed. The lower threshold concentration, however, decreased with increasing test duration from 0.026±0.013μM (9.794±4.897μgL(-1)) to 0.122±0.041μM (40.236±13.75μgL(-1)), respectively, in the 14-days tests. Testing synergy in relation to concentration addition provided the most conservative values. The threshold values for the vertical assessments in tests where the two could be compared were in general 1.2 to 4.7 fold higher than the horizontal assessments. Using passive dosing rather than dilution series or spiking did not lower the threshold significantly. Below the threshold for synergy, slight antagonism could often be observed. This is most likely due to induction of enzymes active in metabolization of alpha-cypermethrin. The results emphasize the importance of test duration when assessing synergy, but also show that azole concentrations within the typically monitored range of up to 0.5μgL(-1) are not likely to cause severe synergy concerning Daphnia magna immobilization.
To assess the exposure to polycyclic aromatic hydrocarbons (PAHs) it is important to understand the binding mechanisms between specific soil constituents and the organic pollutant. In this study, sorptive bioaccessibility extraction (SBE) was applied to quantify the accessible PAH fraction in industrially contaminated soil with and without passive dosing of a competitive sorbate. SBE experiments revealed an accessible PAH fraction of 41 ± 1% (∑16 US EPA PAHs + 5 further PAHs). The passive dosing of toluene below its saturation level revealed competitive binding and resulted in an average increase of the accessible fraction to 49 ± 2%, whereby primarily the accessibility of higher molecular weight PAHs (log Kow > 6) was affected. Competitive binding was verified using the same soil with only desorption-resistant PAHs present. In this experiment, passive dosing of toluene resulted in desorption of 13 ± 0.4% PAH. We explain increased PAH desorption after addition of toluene by competitive adsorption to high-affinity sorption sites while acknowledging that toluene could additionally have increased PAH mobility within the soil matrix. Findings suggest that the presence of copollutants at contaminated sites deserves specific considerations as these may increase accessibility and thereby exposure and mobility of PAHs.

**Enhanced Accessibility of Polycyclic Aromatic Hydrocarbons (PAHs) and Heterocyclic PAHs in Industrially Contaminated Soil after Passive Dosing of a Competitive Sorbate**

To assess the exposure to polycyclic aromatic hydrocarbons (PAHs) it is important to understand the binding mechanisms between specific soil constituents and the organic pollutant. In this study, sorptive bioaccessibility extraction (SBE) was applied to quantify the accessible PAH fraction in industrially contaminated soil with and without passive dosing of a competitive sorbate. SBE experiments revealed an accessible PAH fraction of 41 ± 1% (∑16 US EPA PAHs + 5 further PAHs). The passive dosing of toluene below its saturation level revealed competitive binding and resulted in an average increase of the accessible fraction to 49 ± 2%, whereby primarily the accessibility of higher molecular weight PAHs (log Kow > 6) was affected. Competitive binding was verified using the same soil with only desorption-resistant PAHs present. In this experiment, passive dosing of toluene resulted in desorption of 13 ± 0.4% PAH. We explain increased PAH desorption after addition of toluene by competitive adsorption to high-affinity sorption sites while acknowledging that toluene could additionally have increased PAH mobility within the soil matrix. Findings suggest that the presence of copollutants at contaminated sites deserves specific considerations as these may increase accessibility and thereby exposure and mobility of PAHs.

**General information**

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Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Natural Resources and Life Sciences, Vienna (BOKU)

Contributors: Humel, S., Nørgaard Schmidt, S., Sumetzberger-Hasinger, M., Mayer, P., Loibner, A. P.

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- BFI (2016): BFI-level 2
Microplastics as Vectors for Environmental Contaminants: Exploring Sorption, Desorption, and Transfer to Biota

The occurrence and effects of microplastics (MPs) in the aquatic environment are receiving increasing attention. In addition to their possible direct adverse effects on biota, the potential role of MPs as vectors for hydrophobic organic chemicals (HOCs), compared to natural pathways, is a topic of much debate. It is evident, however, that temporal and spatial variations of MP occurrence do (and will) occur. To further improve the estimations of the role of MPs as vectors for HOC transfer into biota under varying MP concentrations and environmental conditions, it is important to identify and understand the governing processes. Here, we explore HOC sorption to and desorption from MPs and the underlying principles for their interactions. We discuss intrinsic and extrinsic parameters influencing these processes and focus on the importance of the exposure route for diffusive mass transfer. Also, we outline research needed to fill knowledge gaps and improve model-based calculations of MP-facilitated HOC transfer in the environment. Integr Environ Assess Manag 2017;13:488–493. © 2017 SETAC
Partitioning of hydrophobic organic contaminants between polymer and lipids for two silicones and low density polyethylene

Polymers are increasingly used for passive sampling of neutral hydrophobic organic substances (HOC) in environmental media including water, air, soil, sediment and even biological tissue. The equilibrium concentration of HOC in the polymer can be measured and then converted into equilibrium concentrations in other (defined) media, which however requires appropriate polymer to media partition coefficients. We determined thus polymer-lipid partition coefficients (KPL) of various PCB, PAH and organochlorine pesticides by equilibration of two silicones and low density polyethylene (LDPE) with fish oil and Triolein at 4 °C and 20 °C. We observed (i) that KPL was largely independent of lipid type and temperature, (ii) that lipid diffusion rates in the polymers were higher compared to predictions based on their molecular volume, (iii) that silicones showed higher lipid diffusion and lower lipid sorption compared to LDPE and (iv) that absorbed lipid behaved like a co-solute and did not affect the partitioning of HOC at least for the smaller molecular size HOC. The obtained KPL can convert measured equilibrium concentrations in passive sampling polymers into equilibrium concentrations in lipid, which then can be used (1) for environmental quality monitoring and assessment, (2) for thermodynamic exposure assessment and (3) for assessing the linkage between passive sampling and the traditionally measured lipid-normalized concentrations in biota. LDPE-lipid partition coefficients may also be of use for a thermodynamically sound risk assessment of HOC contained in microplastics.
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.04 SJR 1.497 SNIP 1.567
Web of Science (2015): Impact factor 3.698
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.76 SJR 1.59 SNIP 1.639
Web of Science (2014): Impact factor 3.34
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.92 SJR 1.721 SNIP 1.751
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Scopus rating (2012): CiteScore 3.5 SJR 1.794 SNIP 1.618
Web of Science (2012): Impact factor 3.137
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.61 SJR 1.962 SNIP 1.508
Web of Science (2011): Impact factor 3.206
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.879 SNIP 1.424
Web of Science (2010): Impact factor 3.155
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.842 SNIP 1.572
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.658 SNIP 1.58
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.5 SNIP 1.605
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.418 SNIP 1.673
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Scopus rating (2005): SJR 1.479 SNIP 1.558
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Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.902 SNIP 1.06
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.924 SNIP 0.978
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Web of Science (2000): Indexed yes
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Passive dosing of triclosan in multi-generation tests with copepods - Stable exposure concentrations and effects at the low µg L⁻¹ range

Ecotoxicity testing is a crucial component of chemical risk assessment. Still, due to methodological difficulties related to controlling exposure concentrations over time, data on long-term effects of organic chemicals at low concentrations are limited. The aim of the present study was therefore to test the applicability of passive dosing to maintain stable concentrations of the organochlorine bacteriocide triclosan in the water phase during a 6-week multi-generation population development test with the harpacticoid copepod Nitocra spinipes. Triclosan was loaded into silicone (1000 mg), which was used as passive dosing phase in the exposure vials. The distribution ratio for triclosan between silicone and water (D_{silicone-water}) was 10466 ± 1927. A population development test was conducted at three concentration levels of triclosan that were measured to be 3-5 µg L⁻¹, 7-11 µg L⁻¹ and 16-26 µg L⁻¹. Our results demonstrate that passive dosing is applicable for long-term ecotoxicity testing of organic chemicals, including during significant growth of the test organism population. Shifts in the demographic structure of the population during exposure suggest the most severe effects were exerted on juvenile development. Progressively lower development index values in the populations exposed to increasing triclosan concentrations suggest developmental retardation. Our results further stress the need for chronic exposure during ecotoxicity testing in chemical risk assessment as even the most sensitive endpoint was not significant until after 7 days of exposure. This article is protected by copyright. All rights reserved.

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, Stockholm University
Contributors: Ribbenstedt, A., Mustajärvi, L., Breitholtz, M., Gorokhova, E., Mayer, P., Sobek, A.
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Web of Science (2017): Indexed yes
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3 SJR 1.433 SNIP 1.056
Web of Science (2015): Impact factor 2.763
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.89 SJR 1.501 SNIP 1.12
Web of Science (2014): Impact factor 3.225
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.88 SJR 1.656 SNIP 1.086
Web of Science (2013): Impact factor 2.826
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
A passive dosing method to determine fugacity capacities and partitioning properties of leaves

The capacity of leaves to take up chemicals from the atmosphere and water influences how contaminants are transferred into food webs and soil. We provide a proof of concept of a passive dosing method to measure leaf/polydimethylsiloxane partition ratios (Kleaf/PDMS) for intact leaves, using polychlorinated biphenyls (PCBs) as model chemicals. Rhododendron leaves held in contact with PCB-loaded PDMS reached between 76 and 99% of equilibrium within 4 days for PCBs 3, 4, 28, 52, 101, 118, 138 and 180. Equilibrium Kleaf/PDMS extrapolated from the uptake kinetics measured over 4 days ranged from 0.075 (PCB 180) to 0.371 (PCB 3). The Kleaf/PDMS data can readily be converted to fugacity capacities of leaves (Zleaf) and subsequently leaf/water or leaf/air partition ratios (Kleaf/water and Kleaf/air) using partitioning data from the literature. Results of our measurements are within the variability observed for plant/air partition ratios (Kplant/air) found in the literature. Log Kleaf/air from this study ranged from 5.00 (PCB 3) to 8.30 (PCB 180) compared to log Kplant/air of 3.31 (PCB 3) to 8.88 (PCB 180) found in the literature. The method we describe could provide data to characterize the
variability in sorptive capacities of leaves that would improve descriptions of uptake of chemicals by leaves in multimedia fate models.

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Scopus rating (2017): CiteScore 2.84 SJR 1.118 SNIP 0.933
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 1.036 SNIP 0.967
Web of Science (2016): Impact factor 2.592
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.5 SJR 0.998 SNIP 0.923
Web of Science (2015): Impact factor 2.401
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.21 SJR 1.051 SNIP 1.047
Web of Science (2014): Impact factor 2.179
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.996 SNIP 0.949
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ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.023 SNIP 0.87
Web of Science (2012): Impact factor 2.085
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.954 SNIP 0.898
Web of Science (2011): Impact factor 1.991
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.994 SNIP 0.712
Web of Science (2010): Impact factor 1.81
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.092 SNIP 0.977
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.884 SNIP 0.898
Scopus rating (2007): SJR 0.778 SNIP 0.878
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.74 SNIP 0.806
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.745 SNIP 0.878
Scopus rating (2004): SJR 0.692 SNIP 0.782
Scopus rating (2003): SJR 0.502 SNIP 0.706
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Biodegradation of volatile hydrocarbons in five surface waters tested as composed mixtures in the μg/L range

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Combining Equilibrium Sampling with Non-Target Analysis of Hydrophobic Complex Mixtures in a Complex Matrix

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Equilibrium sampling in a semi in situ pot experiment to measure freely dissolved concentrations of hydrophobic organic compounds

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How to Determine the Environmental Exposure of PAHs Originating from Biochar
Biochars are obtained by pyrolyzing biomass materials and are increasingly used within the agricultural sector. Owing to the production process, biochars can contain polycyclic aromatic hydrocarbons (PAHs) in the high mg/kg range, which makes the determination of the environmental exposure of PAHs originating from biochars relevant. However, PAH sorption to biochar is characterized by very high (104–106 L/kg) or extreme distribution coefficients (KD) (>106 L/kg), which makes the determination of exposure scientifically and technically challenging. Cyclodextrin extractions, sorptive bioaccessibility extractions, Tenax extractions, contaminant traps, and equilibrium sampling were assessed and selected methods used for the determination of bioavailability parameters for PAHs in two model biochars. Results showed that: (1) the KD values of typically 106–109 L/kg made the biochars often act as sinks, rather than sources, of PAHs. (2) Equilibrium sampling yielded freely dissolved concentrations (pg–ng/L range) that were below or near environmental background levels. (3) None of the methods were found to be suitable for the direct measurement of the readily desorbing fractions of PAHs (i.e., bioaccessibility) in the two biochars. (4) The contaminant-trap method yielded desorption-resistant PAH fractions of typically 90–100%, implying bioaccessibility in the high μg/kg to low mg/kg range.

General information
Including Bioconcentration Kinetics for thePrioritization and Interpretation of Regulatory Aquatic Toxicity Tests of Highly
Hydrophobic Chemicals

Worldwide, regulations of chemicals require short-term toxicity data for evaluating hazards and risks of the chemicals. Current data requirements on the registration of chemicals are primarily based on tonnage and do not yet consider properties of chemicals. For example, short-term ecotoxicity data are required for chemicals with production volume greater than 1 or 10 ton/y according to REACH, without considering chemical properties. Highly hydrophobic chemicals are characterized by low water solubility and slow bioconcentration kinetics, which may hamper the interpretation of short-term toxicity experiments. In this work, internal concentrations of highly hydrophobic chemicals were predicted for standard acute ecotoxicity tests at three trophic levels, algae, invertebrate, and fish. As demonstrated by comparison with maximum aqueous concentrations at water solubility, chemicals with an octanol-water partition coefficient (Kow) greater than 10^6 are not expected to reach sufficiently high internal concentrations for exerting effects within the test duration of acute tests with fish and invertebrates, even though they might be intrinsically toxic. This toxicity cutoff was explained by the slow uptake, i.e., by kinetics, not by thermodynamic limitations. Predictions were confirmed by data entries of the OECD’s screening information data set (SIDS) (n = 746), apart from a few exceptions concerning mainly organometallic substances and those with inconsistency between water solubility and Kow. Taking error propagation and model assumptions into account, we thus propose a revision of data requirements for highly hydrophobic chemicals with log Kow > 7.4: Short-term toxicity tests can be limited to algae that generally have the highest uptake rate constants, whereas the primary focus of the assessment should be on persistence, bioaccumulation, and long-term effects.
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Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
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Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.86 SNIP 1.809
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.96 SNIP 1.935
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.774 SNIP 1.914
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.55 SNIP 1.893
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.608 SNIP 1.999
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.86 SNIP 2.046
Limited recovery of soil microbial activity after transient exposure to gasoline vapors

During gasoline spills complex mixtures of toxic volatile organic compounds (VOCs) are released to terrestrial environments. Gasoline VOCs exert baseline toxicity (narcosis) and may thus broadly affect soil biota. We assessed the functional resilience (i.e. resistance and recovery of microbial functions) in soil microbial communities transiently exposed to gasoline vapors by passive dosing via headspace for 40 days followed by a recovery phase of 84 days. Chemical exposure was characterized with GC-MS, whereas microbial activity was monitored as soil respiration (CO2 release) and soil bacterial growth ([3H]leucine incorporation). Microbial activity was strongly stimulated and inhibited at low and high exposure levels, respectively. Microbial growth efficiency decreased with increasing exposure, but rebounded during the recovery phase for low-dose treatments. Although benzene, toluene, ethylbenzene and xylene (BTEX) concentrations decreased by 83-97% during the recovery phase, microbial activity in high-dose treatments did not recover and numbers of viable bacteria were 3-4 orders of magnitude lower than in control soil. Re-inoculation with active soil microorganisms failed to restore microbial activity indicating residual soil toxicity, which could not be attributed to BTEX, but rather to mixture toxicity of more persistent gasoline constituents or degradation products. Our results indicate a limited potential for functional recovery of soil microbial communities after transient exposure to high, but environmentally relevant, levels of gasoline VOCs which therefore may compromise ecosystem services provided by microorganisms even after extensive soil VOC dissipation.

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Contributors: Modrzyński, J. J., Christensen, J. H., Mayer, P., Brandt, K. K.
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Web of Science (2016): Impact factor 5.099
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Scopus rating (2015): CiteScore 4.72 SJR 2.003 SNIP 1.75
Microscale In Vitro Assays for the Investigation of Neutral Red Retention and Ethoxyresorufin-O-Deethylase of Biofuels and Fossil Fuels

Only few information on the potential toxic effectiveness of biofuels are available. Due to increasing worldwide demand for energy and fuels during the past decades, biofuels are considered as a promising alternative for fossil fuels in the transport sector. Hence, more information on their hazard potentials are required to understand the toxicological impact of biofuels on the environment. In the German Cluster of Excellence “Tailor-made Fuels from Biomass” design processes for economical, sustainable and environmentally friendly biofuels are investigated. In an unique and interdisciplinary approach, ecotoxicological methods are applied to gain information on potential adverse environmental effects of biofuels at an early phase of their development. In the present study, three potential biofuels, ethyl levulinate, 2-methyltetrahydronorafuran and 2-methylfuran were tested. Furthermore, we investigated a fossil gasoline fuel, a fossil diesel fuel and an established biodiesel. Two in vitro bioassays, one for assessing cytotoxicity and one for aryl hydrocarbon receptor agonism, so called dioxin-like activity, as measured by Ethoxyresorufin-O-Deethylase, were applied using the permanent fish liver cell line RTL-W1 (Oncorhynchus mykiss). The special properties of these fuel samples required modifications of the test design. Points that had to be addressed were high substance volatility, material compatibility and low solubility. For testing of gasoline, diesel and biodiesel, water accommodated fractions and a passive dosing approach were tested to address the high hydrophobicity and low solubility of these complex mixtures. Further work has to focus on an improvement of the chemical analyses of the fuel samples to allow a better comparison of any effects of fossil fuels and biofuels.
Multiple coating thicknesses for sampling of organic pollutants – linear regressions confirm equilibrium even in challenging environmental media

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Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Copenhagen, Aarhus University, Helmholtz Centre for Environmental Research
Contributors: Mayer, P., Nørgaard Schmidt, S., Knudsmark Sjøholm, K., Christensen, J. H., Gidley, P., Vorkamp, K., Witt, G., Jahnke, A.
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Passive Sampling in Regulatory Chemical Monitoring of Nonpolar Organic Compounds in the Aquatic Environment

We reviewed compliance monitoring requirements in the European Union, the United States, and the Oslo-Paris Convention for the protection of the marine environment of the North-East Atlantic, and evaluated if these are met by passive sampling methods for nonpolar compounds. The strengths and shortcomings of passive sampling are assessed for water, sediments, and biota. Passive water sampling is a suitable technique for measuring concentrations of freely dissolved compounds. This method yields results that are incompatible with the EU's quality standard definition in terms of total concentrations in water, but this definition has little scientific basis. Insufficient quality control is a present weakness of passive sampling in water. Laboratory performance studies and the development of standardized methods are needed to improve data quality and to encourage the use of passive sampling by commercial laboratories and monitoring agencies. Successful prediction of bioaccumulation based on passive sampling is well documented for organisms at the lower trophic levels, but requires more research for higher levels. Despite the existence of several knowledge gaps, passive sampling presently is the best available technology for chemical monitoring of nonpolar organic compounds. Key issues to be addressed by scientists and environmental managers are outlined.

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
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BFI (2014): BFI-level 2
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Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Polymers as reference partitioning phase: polymer calibration for an analytically operational approach to quantify multimedia phase partitioning

Polymers are increasingly applied for the enrichment of hydrophobic organic chemicals (HOCs) from various types of samples and media in many analytical partitioning-based measuring techniques. We propose using polymers as a reference partitioning phase and introduce polymer-polymer partitioning as the basis for a deeper insight into partitioning differences of HOCs between polymers, calibrating analytical methods, and consistency checking of existing and calculation of new partition coefficients. Polymer-polymer partition coefficients were determined for polychlorinated...
biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), and organochlorine pesticides (OCPs) by equilibrating 13 silicones, including polydimethylsiloxane (PDMS) and low-density polyethylene (LDPE) in methanol-water solutions. Methanol as cosolvent ensured that all polymers reached equilibrium while its effect on the polymers' properties did not significantly affect silicone-silicone partition coefficients. However, we noticed minor cosolvent effects on determined polymer-polymer partition coefficients. Polymer-polymer partition coefficients near unity confirmed identical absorption capacities of several PDMS materials, whereas larger deviations from unity were indicated within the group of silicones and between silicones and LDPE. Uncertainty in polymer volume due to imprecise coating thickness or the presence of fillers was identified as the source of error for partition coefficients. New polymer-based (LDPE-lipid, PDMS-air) and multimedia partition coefficients (lipid-water, air-water) were calculated by applying the new concept of a polymer as reference partitioning phase and by using polymer-polymer partition coefficients as conversion factors. The present study encourages the use of polymer-polymer partition coefficients, recognizing that polymers can serve as a linking third phase for a quantitative understanding of equilibrium partitioning of HOCs between any two phases.

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Organisations: National Food Institute, Research Group for Molecular Toxicology, Department of Environmental Engineering, Environmental Chemistry, Hamburg University of Applied Sciences, Masaryk University
Contributors: Gilbert, D., Witt, G., Smedes, F., Mayer, P.
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 6.08
Web of Science (2016): Impact factor 6.32
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6
Web of Science (2015): Impact factor 5.886
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.79
Web of Science (2014): Impact factor 5.636
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.01
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Web of Science (2013): Indexed yes
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Scopus rating (2012): CiteScore 5.8
Web of Science (2012): Impact factor 5.695
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
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Scopus rating (2011): CiteScore 5.86
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Remediation of PCB contaminated sediments using activated carbon: Assessing efficiency and robustness using equilibrium sampling

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Remediation of PCB contaminated sediments using activated carbon: Thermodynamic exposure assessment

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Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017
Mixtures of organic contaminants are ubiquitous in the environment. Depending on their persistence and physicochemical properties, individual chemicals that make up the mixture partition and distribute within the environment and might then jointly elicit toxicological effects. For the assessment and monitoring of such mixtures, a variety of cell-based in vitro and low-complexity in vivo bioassays based on algae, daphnids or fish embryos are available. A very important and sometimes unrecognized challenge is how to combine sampling, extraction and dosing to transfer the mixtures from the environment into bioassays, while conserving (or re-establishing) their chemical composition at adjustable levels for concentration-effect assessment. This article outlines various strategies for quantifiable transfer from environmental samples including water, sediment, and biota into bioassays using total extraction or polymer-based passive sampling combined with either solvent spiking or passive dosing.
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Web of Science (2015): Impact factor 5.393
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BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Web of Science (2012): Impact factor 5.257
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
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Web of Science (2011): Impact factor 5.228
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.979 SNIP 1.726
Web of Science (2010): Impact factor 4.827
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.86 SNIP 1.809
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 2.96 SNIP 1.935
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.774 SNIP 1.914
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.55 SNIP 1.893
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.608 SNIP 1.999
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.86 SNIP 2.046
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.54 SNIP 2.065
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Scopus rating (2002): SJR 2.392 SNIP 1.949
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Strategies for transferring mixtures of organic contaminants from multimedia environments into bioassays

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Organisations: Department of Environmental Engineering, Environmental Chemistry, Helmholtz Centre for Environmental Research
Contributors: Jahnke, A., Mayer, P., Schaefer, S., Witt, G., Haase, N., Escher, B.
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Transferring in vivo exposure into in vitro assays using silicone to assess the endocrine activity of POPs accumulated in human breast implants

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Organisations: Department of Environmental Engineering, Environmental Chemistry, National Food Institute, Research Group for Analytical Food Chemistry, Copenhagen Center for Health Technology
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Utilizing the partitioning properties of silicone for the passive sampling of polychlorinated biphenyls (PCBs) in indoor air

The former use of polychlorinated biphenyls (PCBs) in construction materials can lead to elevated indoor air concentrations. We studied the partitioning of PCB congeners between indoor air and silicone with a view to establish passive sampling of PCBs. The release of PCB congeners from silicone followed first order kinetics and confirmed air-side rate-limited mass transfer. Logarithmic elimination rate constants decreased linearly with the logKOA values of the PCB congeners, but varied in a non-linear way with air velocity. Linear uptake of PCBs was found for silicone disks (0.5 mm thickness) in a petri dish, while PCBs reached equilibrium in silicone-coated paper sheets (0.001 mm silicone on each side) exposed to indoor air for 1–2 weeks. The ratios of equilibrium concentrations in silicone and conventionally measured air concentrations were roughly comparable with silicone-air partition coefficients, but further research is required for the determination of silicone-air partition coefficients. Avoiding performance reference compounds (PRCs) because of the indoor setting, the two formats were calibrated against conventional active measurements. Comparisons of air concentrations derived from active and kinetic passive sampling showed a divergence by factors of 2.4 and 2.0 (median values) for the petri dishes and the silicone-coated paper, respectively. With promising results for sensitivity and
precision, the calibration of kinetic passive samplers remains the main challenge and will need suitable, non-hazardous PRCs. Equilibrium sampling indicated promising alternatives.
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.658 SNIP 1.58
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.5 SNIP 1.605
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Scopus rating (2006): SJR 1.418 SNIP 1.673
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.479 SNIP 1.558
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.627 SNIP 1.479
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.321 SNIP 1.323
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.902 SNIP 1.06
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.924 SNIP 0.978
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.959 SNIP 0.871
Web of Science (2000): Indexed yes
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Aged spiked soils cannot resemble desorption and bioaccessibility of native PAHs in historically contaminated soils
In the present study, 25 Austrian soils were collected and spiked with four selected polycyclic aromatic compounds.
Using the contaminant trap, PAH desorption behaviour from freshly contaminated and aged soils was monitored and then compared with three historically PAH-contaminated soils. The aim was to determine fundamental differences in desorption behaviour between spiked and native PAHs. Desorption of PAHs was determined for ground and non-ground samples of historically contaminated soils since increased desorption from ground samples would indicate physical entrapment of PAHs. Desorption experiments were repeated at high additions of toluene since increased desorption in the presence of toluene would indicate competitive binding, which is consistent with adsorption to high affinity sides. Substantial differences were observed between PAH desorption curves for historically polluted soils and spiked soils, and aging of spiked soils was not able to reduce this difference. The bioaccessible PAH fraction was at least one order of magnitude larger in spiked soils compared to real world samples from historically contaminated sites. The observed differences could not be explained by physical entrapment of PAHs in historically contaminated soils since grinding of these soils did not enhance PAH desorption from the soils. The addition of high amounts of toluene to historically contaminated soil resulted in enhanced PAH desorption and a lower desorption resistant fraction. This observation is in line with competitive binding to high affinity sorption sites being the governing retention mechanisms of native PAHs in historically contaminated soils. These results are consistent with two sorption mechanisms occurring in the two types of soils: In historically contaminated soils, PAHs appear to be bound to high affinity sorption sites. A much lower retention in spiked soils is consistent with sorption to a much larger population of low affinity sorption sites. This has important implications for real world situations. It challenges the significance of extrapolations of desorption and bioavailability results that were obtained with PAH spiked soils. Further, a much higher PAH retention in historically contaminated soils suggests limited mobility and exposure of native PAHs. However, the addition of co-solutes can reduce this retention and as a consequence, lead to a re-mobilisation of PAHs.

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Natural Resources and Life Sciences, Vienna (BOKU)
Contributors: Loibner, A. P., Scherr, K. E., Edelmann, E., Humel, S., Kopp, D., Mayer, P.
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A high throughput passive dosing format for the Fish Embryo Acute Toxicity test

High throughput testing according to the Fish Embryo Acute Toxicity (FET) test (OECD Testing Guideline 236) is usually conducted in well plates. In the case of hydrophobic test substances, sorptive and evaporative losses often result in declining and poorly controlled exposure conditions. Therefore, our objective was to improve exposure conditions in FET tests by evaluating a passive dosing format using silicone O-rings in standard 24-well polystyrene plates. We exposed zebrafish embryos to a series of phenanthrene concentrations until 120 h post fertilization (hpf), and obtained a linear dilution series. We report effect values for both mortality and sublethal morphological effects based on (1) measured exposure concentrations, (2) (lipid normalized) body residues and (3) chemical activity. The LC50 for 120 hpf was 310 μg/L, CBR50 (critical body residue) was 2.72 mmol/kg fresh wt and La50 (lethal chemical activity) was 0.047. All values were within ranges expected for baseline toxicity. Impaired swim bladder inflation was the most pronounced morphological effect and swimming activity was reduced in all exposure concentrations. Further analysis showed that the effect on swimming activity was not attributed to impaired swim bladder inflation, but rather to baseline toxicity. We conclude that silicone O-rings (1) produce a linear dilution series of phenanthrene in the 120 hpf FET test, (2) generate and maintain aqueous concentrations for reliable determination of effect concentrations, and allow for obtaining mechanistic toxicity information, and (3) cause no toxicity, demonstrating its potential as an extension of the FET test when testing hydrophobic chemicals.
Toxicological research in the 1930s gave the first indications of the link between narcotic toxicity and the chemical activity of organic chemicals. More recently, chemical activity has been proposed as a novel exposure parameter that describes the fraction of saturation and that quantifies the potential for partitioning and diffusive uptake. In the present study, more than 2000 acute and chronic algal, aquatic invertebrates and fish toxicity data, as well as water solubility and melting point values, were collected from a series of sources. The data were critically reviewed and grouped by mode of action (MoA). We considered 660 toxicity data to be of acceptable quality. The 328 data which applied to the 72 substances identified as MoA 1 were then evaluated within the activity-toxicity framework: EC50 and LC50 values for all three taxa correlated...
generally well with (subcooled) liquid solubilities. Acute toxicity was typically exerted within the chemical activity range of 0.01-0.1, whereas chronic toxicity was exerted in the range of 0.001-0.01. These results confirm that chemical activity has the potential to contribute to the determination, interpretation and prediction of toxicity to aquatic organisms. It also has the potential to enhance regulation of organic chemicals by linking results from laboratory tests, monitoring and modeling programs. The framework can provide an additional line of evidence for assessing aquatic toxicity, for improving the design of toxicity tests, reducing animal usage and addressing chemical mixtures.

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ISI indexed (2013): ISI indexed yes
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BFI (2011): BFI-level 2
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Web of Science (2011): Impact factor 5.228
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Bioaccessibility Extraction of Hydrophobic Pollutants: Benefits of Separating Leaching Agent and Acceptor Medium

Bioaccessibility extractions of organic pollutants from environmental solid samples are increasingly used in environmental risk assessment and management. Recent research has indicated that many bioaccessibility extraction methods have limited sink capacity for hydrophobic organic chemicals, which can lead to underestimation of bioaccessibility. Therefore, several studies have proposed to add a sink to the extraction medium, including the so called contaminant trap, the silicon rod based sorptive bioaccessibility extraction and tenax beads-assisted extractions. While these methods certainly are a step forward, they also lead to challenges related to the separation of sink and matrix and/or the subsequent quantification of the bioaccessible fraction. The present study aimed at developing a new approach for (1) enhancing the sink capacity of bioaccessibility extraction, (2) improving phase separation and (3) facilitating the measurement of the bioaccessible fraction. Cyclodextrin was used as leaching agent, ethanol as acceptor medium and a semipermeable membrane for separating these two phases. Various physical formats of this configuration were developed and tested, and the simplest and highly performing format was further optimized and validated. This new configuration was characterized in terms of mass transfer kinetics, analytical performance criteria and suitability for direct analysis by high performance liquid chromatography (HPLC) and gas chromatography (GC). Finally, the developed method was applied to PAH contaminated soils and the results compared to results obtained with other existing methods.

General information
Bioaccumulation in aquatic systems: methodological approaches, monitoring and assessment

Bioaccumulation, the accumulation of a chemical in an organism relative to its level in the ambient medium, is of major environmental concern. Thus, monitoring chemical concentrations in biota are widely and increasingly used for assessing the chemical status of aquatic ecosystems. In this paper, various scientific and regulatory aspects of bioaccumulation in aquatic systems and the relevant critical issues are discussed. Monitoring chemical concentrations in biota can be used for compliance checking with regulatory directives, for identification of chemical sources or event-related environmental risk assessment. Assessing bioaccumulation in the field is challenging since many factors have to be considered that can affect the accumulation of a chemical in an organism. Passive sampling can complement biota monitoring since samplers with standardised partition properties can be used over a wide temporal and geographical range. Bioaccumulation is also assessed for regulation of chemicals of environmental concern whereby mainly data from laboratory studies on fish bioaccumulation are used. Field data can, however, provide additional important information for regulators. Strategies for bioaccumulation assessment still need to be harmonised for different regulations and groups of chemicals. To create awareness for critical issues and to mutually benefit from technical expertise and scientific findings, communication between risk assessment and monitoring communities needs to be improved. Scientists can support the establishment of new monitoring programs for bioaccumulation, e.g. in the frame of the amended European Environmental Quality Standard Directive.
Biocides from façade coatings in urban surface waters: Estimating the leaching of biocides from render by polyacrylate-water partitioning constants?

Leaching of biocides from façade coatings attracts more and more attention within recent years. In-can as well as film preserving biocides are added to polymer resin based renders and paints in order protect from microbial spoilage. However, several studies revealed that biocides leach from the façade coating and are detectable in urban stormwater runoff. The present study focussed on the occurrence of biocides in the aqueous environment - both in urban water close to the sources as well as further away in fresh and marine waters. It could be shown that biocides are ubiquitous in the aqueous environment. They are detectable not only close to their sources in stormwater run-off but also further away in marine waters with concentrations up to 60 ng L⁻¹ (mecoprop up to 200 ng L⁻¹). Further work was done in order to estimate the leaching of biocides from building material. The possibility of using polyacrylate-water partition constants in comparison to render-water distribution constants was introduced for this purpose. The results showed that polyacrylate-water partition constants might serve as a useful and practical tool which would be closer to the reality than the commonly used water solubility and octanolwater partition constants.

General information
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Comparison of passive and standard dosing of polycyclic aromatic hydrocarbons to the marine algae Phaeodactylum tricornutum

Testing hydrophobic organic compounds (HOCs), like polycyclic aromatic hydrocarbons (PAHs), in aquatic toxicity tests is difficult due to compound losses through volatilization, sorption to the test vessel and culture medium constituents. This
results in poorly defined exposure, the bioavailable concentration is reduced and concentration-effect-relation might be underestimated. Passive dosing can overcome these problems by the continual partitioning of HOCs from a dominating reservoir loaded in a biologically inert polymer such as silicone. This procedure provides defined and constant freely dissolved concentrations and eliminates spiking with cosolvents. Passive dosing using silicone Orings as donor and PAHs as test substances (fluoranthene, naphthalene, phenanthrene, acenaphthene, fluorene, benzo[a]pyrene, anthracene and pyrene) were applied in the marine algal growth inhibition test with Phaeodactylum tricornutum (based on ISO EN 10253) in 24-well microtiter plates. The O-rings were loaded by partitioning from methanol solutions or suspensions of the respective PAHs (1), and these loaded O-rings were added to the wells in test media before the beginning of the test. Agitation of the plates was used to speed up the release from the O-rings. The toxicity of the individual PAHs was investigated at controlled concentrations up to their aqueous solubility in artificial seawater. The concentration-dependent growth inhibition of Phaeodactylum tricornutum was then compared for passive dosing and standard dosing according to the standard marine algae test procedure on microtiter plates. A comparison of the EC50 values of passive dosing vs. EC50 values of standard dosing showed an underestimation of the effects when using nominal standard dosing probably due to sorption, evaporation and limiting dissolution kinetics. Furthermore, passive dosing concentration-response curves were more reproducible and shifted towards lower concentrations. Results show that the response is clearly not only dependent on the potency of the compounds, but also on its supply, sorption and consumption during the assay. Passive dosing is a practical and economical way of improving the exposure of HOCs in aquatic toxicity or bioconcentration tests like the algae growth inhibition test. vn (1) K. E. C. Smith, N. Domb, R. Blust, P. Mayer (2010) Controlling and maintaining exposure of hydrophobic organic compounds in aquatic toxicity tests by passive dosing.

**General information**

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**Organisations:** Department of Environmental Engineering, Environmental Chemistry, University of Hamburg

**Contributors:** Witt, G., Niehus, N. C., Konopka, K., Mayer, P., Floeter, J.

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**Determining High-Quality Critical Body Residues for Multiple Species and Chemicals by Applying Improved Experimental Design and Data Interpretation Concepts**

Ecotoxicological effect data are generally expressed as effective concentrations in the external exposure medium and do thus not account for differences in chemical uptake, bioavailability, and metabolism, which can introduce substantial data variation. The Critical Body Residue (CBR) concept provides clear advantages, because it links effects directly to the internal exposure. Using CBRs instead of external concentrations should therefore reduce variability. For compounds that act via narcosis even a constant CBR has been proposed. Despite the expected uniformity, CBR values for these compounds still show large variability, possibly due to biased and inconsistent experimental testing. In the present study we tested whether variation in CBR data can be substantially reduced when using an improved experimental design and avoiding confounding factors. The aim was to develop and apply a well-defined test protocol for accurately and precisely measuring CBR data, involving improved (passive) dosing, sampling, and processing of organisms. The chemicals 1,2,4-trichlorobenzene, 1,2,3,4-tetrachlorobenzene, 1,2,3,4,5,6-tetrachloroaniline, 4-chloro-3-methylphenol, pentylbenzene, pyrene, and bromophos-methyl were tested on Lumbriculus varieigatus (California blackworm), Hyalella azteca (scud), and Poecilia reticulata (guppy), which yielded a high-quality database of 348 individual CBR values. Medians of CBR values ranged from 2.1 to 16.1 mmol/kg wet weight (ww) within all combinations of chemicals and species, except for the insecticide bromophos-methyl, for which the median was 1.3 mmol/kg ww. The new database thus covers about one log unit, which is considerably less than in existing databases. Medians differed maximally by a factor of 8.4 between the 7 chemicals but within one species, and by a factor of 2.6 between the three species but for individual chemicals. Accounting for the chemicals internal distribution to different partitioning domains and relating effects to estimated concentrations in the target compartment (i.e., membrane lipids) was expected to but did not decrease the overall variability, likely because the surrogate partition coefficients for membrane lipid, storage lipid, protein, and carbohydrate that were used as input parameters did not sufficiently represent the actual partitioning processes. The results of this study demonstrate that a well-designed test setup can produce CBR data that are highly uniform beyond chemical and biological diversity.

**General information**

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**Organisations:** Department of Environmental Engineering, Environmental Chemistry, Utrecht University, Aarhus University

**Contributors:** van der Heijden, S. A., Hermens, J. L. M., Sinnige, T. L., Mayer, P., Gilbert, D., Jonker, M. T. O.

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Differences between Lipids Extracted from Five Species Are Not Sufficient To Explain Biomagnification of Nonpolar Organic Chemicals

Lipids are the major sorptive phase for many organic chemicals that bioaccumulate in foodwebs. However, "lipids" are usually operationally defined by the extraction protocol. Large differences in sorptive capacities between species would violate assumptions implicit in widely used lipid-normalization procedures and invalidate generic bioaccumulation factors. We extracted lipids from five species from different trophic levels and domains and determined fractions of triglycerides, phospholipids, and cholesterol. We passively dosed the lipids with cyclic volatile methylsiloxanes and chlorobenzenes via headspace from spiked olive oil to determine their sorptive capacities. Lipids from seal blubber and pork bacon solely composed of triglycerides had capacities similar to that of olive oil; lipids from mussels, herring, and guillemot egg had quantifiable fractions of phospholipids and cholesterol and showed capacities reduced by factors of up to 2.3-fold. Generally, the sorptive capacities of the lipids were not elevated relative to the olive oil controls and are unlikely to explain a substantial part of biomagnification.
Differential immunomodulatory responses to nine polycyclic aromatic hydrocarbons applied by passive dosing

Studying the effects of hydrophobic chemicals using in vitro cell based methods is hindered by the difficulty in bringing and keeping these chemicals in solution. Their effective concentrations are often lower than their nominal concentrations. Passive dosing is one approach that provides defined and stable dissolved concentrations during in vitro testing, and was applied to control and maintain freely dissolved concentrations of polycyclic aromatic hydrocarbons (PAHs) at levels up to their aqueous solubility limit. The immunomodulatory effects of 9 different PAHs at aqueous solubility on human bronchial epithelial cells were determined by analysing the cytokine promoter expression of 4 different inflammatory cytokines using stably transfected recombinant A549 cell lines. Diverse immunomodulatory responses were found with the highest induction observed for the most hydrophobic PAHs chrysene, benzo(a)antracene and benzo(a)pyrene. Cytokine promoter expression was then studied in dose response experiments with acenaphthene, phenanthrene and benzo(a)anthracene. The strongest induction was observed for benzo(a)anthracene. Cell viability analysis was performed and showed that none of the PAHs induced cytotoxicity at any of the concentrations tested. Overall, this study shows that (1) immunomodulatory effects of PAHs can be studied in vitro at controlled freely dissolved concentrations, (2) the most hydrophobic PAHs were the strongest inducers and (3) induction was often higher at lower exposure levels and decreased then with concentration despite the apparent absence of cytotoxicity. (C) 2014 Elsevier Ltd. All rights reserved.

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Salzburg, Aarhus University
Contributors: Oostingh, G. J., Smith, K. E. C., Tischler, U., Radauer-Preiml, I., Mayer, P.
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Effect of narcotics on membrane-bound mitochondrial processes in fish

Around 70% of industrial chemicals are hydrophobic compounds which are assumed to elicit toxicity through narcosis by accumulating in membranes and disrupting membrane integrity and function. Although narcosis has been recognized as an important toxicity mechanism for decades, ecotoxicological research has been mostly limited to the development of quantitative structure activity relations (QSARs) to predict toxicity, resulting in insufficient understanding of the exact mechanisms involved. In this study we investigate specific aspects of the mechanism of narcosis in fish using both alternative in vivo (zebrafish embryo) and in vitro tests. We applied a passive dosing method to expose zebrafish embryos up to 5 days post fertilization to linear dilution series of a set of non-polar narcotics (phenanthrene and three chlorobenzene structure analogues). In addition to increasing mortality, we observed decreasing growth, heart rate and motility with increasing exposure concentration of all narcotics, consistent with the general assumption of reduced cardiorespiratory function. At the cellular level, the cell membrane is expected to be the first target of narcotics. Since the mitochondrial and endoplasmic reticulum membrane are known to closely interact with the cell membrane, we hypothesize that narcotics can be further partitioned into these organelle membranes where they can disrupt essential membrane-bound processes. The electron transport chain (ETC) is an example of a crucial mitochondrial membrane-bound process and is therefore a potential target. We found that in zebrafish embryos ETC activity was increased at low exposure concentrations, suggesting a compensatory response, while it decreased when exposure concentrations reached levels causing reduced motility, heart rate and eventually mortality. The effect of narcotic compounds on ETC activity was confirmed in vitro: we observed inhibition of the ETC after adding the compounds directly to a homogenate of control embryos. To further investigate effects on the energy production system, and to characterize the observed compensatory response, we are currently measuring the effect of narcotics on ATP synthase activity both in vivo and directly in vitro. Although narcosis is commonly considered a non-specific mechanism of toxicity acting by membrane disruption in general, we illustrate how we can increase our understanding of narcosis by focussing on specific membrane types and...
membrane-bound processes.

**General information**

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Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Antwerp
Contributors: Vergauwen, L., Nørregaard Schmidt, S., Michiels, E., Stinckens, E., Maho, W., Blust, R., Covaci, A., Mayer, P., Knappen, D.
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**Bibliographical note**

Poster session
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**Endocrine activity of persistent organic pollutants accumulated in human silicone implants — Dosing in vitro assays by partitioning from silicone**

Persistent organic pollutants (POPs) accumulated in human tissues may pose a risk for human health by interfering with the endocrine system. This study establishes a new link between actual human internal POP levels and the endocrine active dose in vitro, applying partitioning-controlled dosing from silicone to the H295R steroidogenesis assay: (1) Measured concentrations of POPs in silicone breast implants were taken from a recent study and silicone disks were loaded according to these measurements. (2) Silicone disks were transferred into H295R cell culture plates in order to control exposure of the adrenal cells by equilibrium partitioning. (3) Hormone production of the adrenal cells was measured as toxicity endpoint. 4-Nonylphenol was used for method development, and the new dosing method was compared to conventional solvent-dosing. The two dosing modes yielded similar dose-dependent hormonal responses of H295R cells. However, with the partitioning-controlled freely dissolved concentrations (Cfree) as dose metrics, dose–response curves were left-shifted by two orders of magnitude relative to spiked concentrations. Partitioning-controlled dosing of POPs resulted in up to 2-fold increases in progestagen and corticosteroid levels at Cfree of individual POPs in or below the femtomolar range. Silicone acted not only as source of the POPs but also as a sorption sink for lipophilic hormones, stimulating the cellular hormone production. Methodologically, the study showed that silicone can be used as reference partitioning phase to transfer in vivo exposure in humans (silicone implants) to in vitro assays (partitioning-controlled dosing). The main finding was that POPs at the levels at which they are found in humans can interfere with steroidogenesis in a human adrenocortical cell line.

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Organisations: National Food Institute, Department of Environmental Engineering, Environmental Chemistry, Research Group for Analytical Food Chemistry, Research Group for Molecular Toxicology, Aarhus University
Contributors: Gilbert, D., Mayer, P., Pedersen, M., Vinggaard, A. M.
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BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.49 SJR 2.544 SNIP 2.125
Web of Science (2015): Impact factor 5.929
Equilibrium passive sampling as a tool to study polycyclic aromatic hydrocarbons in Baltic Sea sediment pore-water systems

Solid Phase Microextraction (SPME) was applied to provide the first large scale dataset of freely dissolved concentrations for 9 polycyclic aromatic hydrocarbons (PAHs) in Baltic Sea sediment cores. Polydimethylsiloxane (PDMS) coated glass fibers were used for ex-situ equilibrium sampling followed by automated thermal desorption and GC–MS analysis. From the PAH concentrations in the fiber coating we examined (i) spatially resolved freely dissolved PAH concentrations \((C_{\text{free}})\); (ii) baseline toxicity potential on the basis of chemical activities \((a)\); (iii) site specific mixture compositions; (iv) diffusion gradients at the sediment water interface and within the sediment cores and (v) site specific distribution ratios.
Contamination levels were low in the northern Baltic Sea, moderate to elevated in the Baltic Proper and highest in the Gulf of Finland. Chemical activities were well below levels expected to cause narcosis to benthos organisms. The SPME method is a very sensitive tool that opens new possibilities for studying the PAHs at trace levels in marine environments.

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, University of the West of Scotland, Leibniz Institute for Baltic Sea Research Warnemunde (IOW), Hamburg University of Applied Sciences
Contributors: Lang, S., Hursthouse, A., Mayer, P., Hand, I., Schulz-Bull, D., Witt, G.
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Scopus rating (2010): SJR 1.292 SNIP 1.282
Web of Science (2010): Impact factor 2.359
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Equilibrium sampling for a thermodynamic assessment of contaminated sediments

Hydrophobic organic contaminants (HOCs) reaching the aquatic environment are largely stored in sediments. The risk of contaminated sediments is challenging to assess since traditional exhaustive extraction methods yield total HOC concentrations, whereas freely dissolved concentrations (C\text{free}) govern diffusive uptake and partitioning. Equilibrium sampling of sediment was introduced 15 years ago to measure C\text{free}, and it has since developed into a straightforward, precise and sensitive approach for determining C\text{free} and other exposure parameters that allow for thermodynamic assessment of polluted sediments. Glass jars with µm-thin silicone coatings on the inner walls can be used for ex situ equilibration while a device housing several silicone-coated fibers can be used for in situ equilibration. In both cases, parallel sampling with varying silicone thicknesses can be applied to confirm valid equilibrium sampling (method incorporated QA/QC). The measured equilibrium concentrations in silicone (C\text{sil}) can then be divided by silicone/water partition ratios to yield C\text{free}. C\text{sil} can also be compared to C\text{sil} from silicone equilibrated with biota in order to determine the equilibrium status of the biota relative to the sediment. Furthermore, concentrations in lipid at thermodynamic equilibrium with sediment (C\text{lip} \times K_{\text{lip}}/C_{\text{sil}}) can be calculated via lipid/silicone partition ratios C\text{sil} × K_{\text{lip}}/C_{\text{sil}}, which has been done in studies with limnic, river and marine sediments. The data can then be compared to lipid-normalized concentrations in aquatic organisms or to regulatory thresholds. Finally, C\text{sil} can also be converted into chemical activities (a), which express the energetic level of the chemicals, drive several spontaneous processes and are well linked to the potential for baseline (mixture) toxicity. This overview lecture will focus at the latest developments in equilibrium sampling concepts and methods. Further, we will explain how these approaches can provide a new basis for a thermodynamic assessment of polluted sediments.

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Organisations: Department of Environmental Engineering, Environmental Chemistry, USACE-ERDC, University of Eastern Finland, Hamburg University of Applied Sciences, German Federal Institute of Hydrology (BfG), Stockholm University
Contributors: Mayer, P., Nørgaard Schmidt, S., Mäenpää, K., Witt, G., Schäfer, S., Gidley, P., Jahnke, A.

Equilibrium sampling for a thermodynamic assessment of contaminated sediments

Hydrophobic organic contaminants (HOCs) reaching the aquatic environment are largely stored in sediments. The risk of contaminated sediments is challenging to assess since traditional exhaustive extraction methods yield total HOC concentrations, whereas freely dissolved concentrations (C\text{free}) govern diffusive uptake and partitioning. Equilibrium sampling of sediment was introduced 15 years ago to measure C\text{free}, and it has since developed into a straightforward, precise and sensitive approach for determining C\text{free} and other exposure parameters that allow for thermodynamic assessment of polluted sediments. Glass jars with µm-thin silicone coatings on the inner walls can be used for ex situ equilibration while a device housing several silicone-coated fibers can be used for in situ equilibration. In both cases, parallel sampling with varying silicone thicknesses can be applied to confirm valid equilibrium sampling (method incorporated QA/QC). The measured equilibrium concentrations in silicone (C\text{sil}) can then be divided by silicone/water partition ratios to yield C\text{free}. C\text{sil} can also be compared to C\text{sil} from silicone equilibrated with biota in order to determine the equilibrium status of the biota relative to the sediment. Furthermore, concentrations in lipid at thermodynamic equilibrium with sediment (C\text{lip} \times K_{\text{lip}}/C_{\text{sil}}) can be calculated via lipid/silicone partition ratios C\text{sil} × K_{\text{lip}}/C_{\text{sil}}, which has been done in studies with limnic, river and marine sediments. The data can then be compared to lipid-normalized concentrations in aquatic organisms or to regulatory thresholds. Finally, C\text{sil} can also be converted into chemical activities (a), which express the energetic level of the chemicals, drive several spontaneous processes and are well linked to the potential for baseline (mixture) toxicity. This overview lecture will focus at the latest developments in equilibrium sampling concepts and methods. Further, we will explain how these approaches can provide a new basis for a thermodynamic assessment of polluted sediments.

General information

State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, USACE-ERDC, University of Eastern Finland, Hamburg University of Applied Sciences, German Federal Institute of Hydrology (BfG), Stockholm University
Contributors: Mayer, P., Nørgaard Schmidt, S., Mäenpää, K., Witt, G., Schäfer, S., Gidley, P., Jahnke, A.

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incorporated QA/QC). The measured equilibrium concentrations in silicone (Csil) can then be divided by silicone/water partition ratios to yield Cfree. Csil can also be compared to Csil from silicone equilibrated with biota in order to determine the equilibrium status of the biota relative to the sediment. Furthermore, concentrations in lipid at thermodynamic equilibrium with sediment (Clip?Sed) can be calculated via lipid/silicone partition ratios Csil × KLip:Sil, which has been done in studies with limnic, river and marine sediments. The data can then be compared to lipid-normalized concentrations in aquatic organisms or to regulatory thresholds. Finally, Csil can also be converted into chemical activities (a), which express the energetic level of the chemicals, drive several spontaneous processes and are well linked to the potential for baseline (mixture) toxicity. This overview lecture will focus at the latest developments in equilibrium sampling concepts and methods. Further, we will explain how these approaches can provide a new basis for a thermodynamic assessment of polluted sediments.

**General information**

State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, USACE-ERDC, University of Eastern Finland, Hamburg University of Applied Sciences, German Federal Institute of Hydrology (BfG), Stockholm University
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**Equilibrium sampling of hydrophobic organic chemicals in sediments: challenges and new approaches**

The exposure risk of contaminated sediments is traditionally assessed by exhaustive extraction methods that measure total concentrations (c total) including bound and freely dissolved contaminants. However, freely dissolved concentrations (c free) of hydrophobic organic chemicals (HOCs) are considered to be the effective concentrations for diffusive uptake and partitioning, and they can be measured by equilibrium sampling. We have thus applied glass jars with multiple coating thicknesses for equilibrium sampling of HOCs in sediment samples from various sites in different German rivers. The coated glass jars were very convenient for routine monitoring campaigns since (1) equilibration times are minimized by the very thin coatings, (2) the equilibration is done in the laboratory and (3) equilibrium sampling is confirmed by equal analyte concentrations in various silicone coating thicknesses without tedious time-serious measurements. However, for some sediment samples analyte concentrations decreased towards thicker silicone coating possibly caused by depletion of the sediment or equilibrium partitioning not being attained. In this study, we investigated the application of sediment depletion and kinetic uptake models. Sediment depletion was tested by the model for multi ratio equilibrium sampling (Smedes et al. ES&T 2013). If non-depletion was assumed by a sufficient capacity ratio between sampler and sediment (< 0.05) and by low hydrophobic PCBs attaining equilibrium, the lower analyte concentrations in thicker silicone coating for more hydrophobic PCBs can be explained by non-equilibrium. Equilibrium concentrations in silicone were then determined by non-linear least square regression of analyte concentrations in polymer as a function of silicone mass using a first order kinetic model. Finally, the model was used to determine c free of PCBs at different sites. Next to non-equilibrium partitioning for some compounds, we had difficulties in detecting target analytes such as p,p′-DDT in coated glass extracts despite high c total in the respective sediment samples. We will demonstrate that microbial degradation can play a significant role during equilibrium sampling of biodegradable compounds even during short incubation times and despite confirmation of equilibrium partitioning.

**General information**

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Organisations: Department of Environmental Engineering, Environmental Chemistry
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Equilibrium sampling can be applied to measure freely dissolved concentrations (C_{free}) of hydrophobic organic chemicals (HOCs) that are considered effective concentrations for diffusive uptake and partitioning. It can also yield concentrations in lipids at thermodynamic equilibrium with the sediment (C_{lip\rightarrow sed}) by multiplying concentrations in the equilibrium sampling polymer with lipid to polymer partition coefficients. We have applied silicone coated glass jars for equilibrium sampling of seven 'indicator' polychlorinated biphenyls (PCBs) in sediment samples from ten locations along the River Elbe to measure C_{lip\rightarrow sed} of PCBs and their C_{bio,lip} that were determined independently by the German Environmental Specimen Bank in common bream, a fish species living in close contact with the sediment: (1) In all cases, C_{bio,lip} were below C_{lip\rightarrow sed}, (2) there was proportionality between the two parameters with high R^2 values (0.92–1.00) and (3) the slopes of the linear regressions were very similar between the three stations (0.297; 0.327; 0.390). These results confirm the close link between PCB bioaccumulation and the thermodynamic potential of sediment-associated HOCs for partitioning into lipids. This novel approach gives clearer and more consistent results compared to conventional approaches that are based on total concentrations in sediment and biota-sediment accumulation factors. We propose to apply equilibrium sampling for determining bioavailability and bioaccumulation potential of HOCs, since this technique can provide a thermodynamic basis for the risk assessment and management of contaminated sediments.

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, German Federal Institute of Hydrology (BfG)
Contributors: Schäfer, S., Antoni, C., Möhlenkamp, C., Claus, E., Reifferscheid, G., Heininger, P., Mayer, P.
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Web of Science (2006): Indexed yes
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Web of Science (2004): Indexed yes
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Web of Science (2003): Indexed yes
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Erratum to: Bioaccumulation in aquatic systems: methodological approaches, monitoring and assessment

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry
Number of pages: 1
Publication date: 2015
Fate of polychlorinated biphenyls in a contaminated lake ecosystem: Combining equilibrium passive sampling of sediment and water with total concentration measurements of biota: Chemical equilibrium status of an aquatic ecosystem

Equilibrium sampling devices can be applied to study and monitor the exposure and fate of hydrophobic organic chemicals on a thermodynamic basis. They can be used to determine freely dissolved concentrations and chemical activity ratios and to predict equilibrium partitioning concentrations of hydrophobic organic chemicals in biota lipids. The authors’ aim was to assess the equilibrium status of polychlorinated biphenyls (PCBs) in a contaminated lake ecosystem and along its discharge course using equilibrium sampling devices for measurements in sediment and water and by also analyzing biota. The authors used equilibrium sampling devices (silicone rubber and polyethylene [PE]) to determine freely dissolved concentrations and chemical activities of PCBs in the water column and sediment porewater and calculated for both phases the corresponding equilibrium concentrations and chemical activities in model lipids. Overall, the studied ecosystem appeared to be in disequilibrium for the studied phases: sediment, water, and biota. Chemical activities of PCBs were higher in sediment than in water, which implies that the sediment functioned as a partitioning source of PCBs and that net diffusion occurred from the sediment to the water column. Measured lipid-normalized PCB concentrations in biota were generally below equilibrium lipid concentrations relative to the sediment (CLip ⇌Sed ) or water (CLip ⇌W ), indicating that PCB levels in the organisms were below the maximum partitioning levels. The present study shows the application versatility of equilibrium sampling devices in the field and facilitates a thermodynamic understanding of
exposure and fate of PCBs in a contaminated lake and its discharge course. Environ Toxicol Chem 2015;34:2463-2474. © 2015 SETAC.

**General information**

**State:** Published

**Organisations:** Department of Environmental Engineering, Environmental Chemistry, University of Eastern Finland, Aarhus University, Helmholtz Centre for Environmental Research, Finnish Environment Institute

**Contributors:** Mäenpää, K., Leppänen, M. T., Figueiredo, K., Mayer, P., Gilbert, D., Jahnke, A., Gil-Allué, C., Akkanen, J., Nybom, I., Herve, S.

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- Scopus rating (2011): CiteScore 3.05 SJR 1.947 SNIP 1.168
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- Web of Science (2011): Indexed yes
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- Scopus rating (2010): SJR 1.715 SNIP 0.992
- Web of Science (2010): Impact factor 3.026
- Web of Science (2010): Indexed yes
Foundational aspects of the concept of chemical activity

The chemical activity of an organic chemical quantifies its potential for spontaneous physicochemical processes, such as diffusion, sorption, and partitioning. For instance, the chemical activity of a sediment contaminant determines its equilibrium partitioning concentration in sediment-dwelling organisms and differences in chemical activity determine the direction and extent of diffusion between environmental compartments [1,2]. This makes chemical activity a meaningfull and well-defined exposure parameter that is closely linked to fugacity and freely dissolved concentration [2]. Classical toxicological studies have provided the first indication that narcosis occurs within a relatively narrow band of chemical activity [3-5], and during the last 10 years several studies have confirmed this for the „baseline toxicity“ of non-polar organic chemicals and their mixtures [6-8].

The first aim of this presentation will be to emphasize the physical meaning of chemical activity, basically suggesting that „mass concentration“ and „chemical activity“ are two complentary dimensions for chemicals in the environment, exactly like we know from other areas (heat content versus temperature; water content versus water activity). The second aim will be to present how chemical activity can be measured and controlled in environmental research and testing, since this has the very important implication that chemical activity goes beyond modelling and re-calculations of mass based data. The final aim will be to initiate the discussion of why and how „chemical activity“ can help (1) to link exposure between media, (2) to compare sensitivities between species, (3) to assess (excess) toxicity of chemicals and (4) to add up the exposure for mixtures?

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Contributors: Mayer, P.
Pages: 14-14
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How do non-specific mechanisms of toxicity fit into the AOP framework? The example of narcosis

Adverse Outcome Pathway (AOP) development is currently being formalized around a set of internationally harmonized principles. While these principles can often be applied in a relatively straightforward manner in cases in which the sequence of key events (KEs) is fairly specific, defining and describing appropriate re-usable KEs can be particularly challenging when relatively non-specific toxicological mechanisms are involved. A well-known example of such a non-specific mechanism is membrane disruption through narcosis, which is commonly accepted to result from accumulation of lipophilic chemicals in membranes disrupting membrane integrity and function. It has been difficult to delineate a complete AOP for narcosis, resulting in insufficient understanding of the exact mechanisms involved to e.g. support robust read across groupings based on mechanism of action. We summarized the two main pathways that have been described for narcosis in a hypothesized AOP. The first outlines a generalized pathway leading to a loss of equilibrium and mortality at the organismal level through changes in cellular respiration and metabolic rate. The second focused on disruption of epithelium of primary and secondary gill lamellae resulting in pathologic alterations, ultimately causing hypoxia and respiratory failure. We applied a passive dosing method to expose zebrafish embryos up to 5 days to a linear dilution series of phenanthrene. We observed reduced survival (LC 50: 310.0 μg/l), and reduced growth with increasing accumulated dose. We observed that the distance travelled was significantly reduced in all phenanthrene exposure concentrations. We found that while exposed larvae were able to reach high swim speeds (> 10 mm/s), they travelled less distance at these high speeds. We also found that impaired inflation of the posterior swim bladder chamber was the most important sublethal morphological effect after phenanthrene exposure. One could expect that the reduced swimming activity is caused by the failure to inflate the swim bladder. However, the effect of impaired swim bladder inflation on swimming activity was small relative to the narcosis effect. Currently, we are defining underlying key events leading to these adverse outcomes. We are currently in the process of determining the distribution of narcotic compounds across different membrane types (cell membrane versus mitochondrial membrane), and of evaluating in vitro tools for the assessment of narcotic effects.

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Linking algal growth inhibition to chemical activity

Unitless chemical activity, expressing the energetic level of a compound relative to its energetic level in pure liquid [0-1], has proven useful to quantify the effective exposure to hydrophobic organic compounds through both aerial and aqueous media. Several studies have linked toxicity to chemical activity, as opposed to e.g. the total concentration. Baseline toxicity (narcosis) for neutral hydrophobic organic compounds has been shown to initiate in the narrow chemical activity range of 0.01 to 0.1. This presentation focuses on linking algal growth inhibition to chemical activity with the aims to (1) further challenge the current chemical activity range for baseline toxicity, and (2) extend the utilisation of the chemical activity concept across compounds and species. The first part of the presentation focuses on results from a recently published study, in which toxicity data for 39 non-polar liquids were applied to challenge the chemical activity range for baseline toxicity. For each compound, the effective activity (Ea50) was estimated as the ratio of the effective concentration (EC50) and water solubility. Of these ratios, 90% were within the expected chemical activity range of 0.01 to 0.1 for baseline toxicity, and none of the ratios were significantly below 0.01. On a practical level, these findings suggest EC50 values for baseline toxicity to be at or above 1% of water solubility. On an environmental risk assessment level, predicted no-effect concentrations (PNECs) for baseline toxicity could even be set as a percentage of saturation, and this approach can easily be extended to baseline toxicity of mixtures. However, EC50 values well below 1% of saturation can still occur and indicate the potential for excess toxicity through a specific or reactive mode of action. The second part of the presentation focuses on extending the utilisation of the chemical activity concept. More specifically, the chemical activity concept is applied to a much larger range of algal toxicity data, including a wide range of solids and liquids, covering several expected modes of action and also several algal species. High-quality toxicity data are carefully selected from peer-
reviewed scientific literature and QSAR databases. This presentation shows how the chemical activity concept can be used to compare and combine toxicity data across compounds and species in order to characterize toxicity – and further how the concept can be used in environmental risk assessment.

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Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2015

**Linking algal growth inhibition to chemical activity - Baseline toxicity required 1% of saturation**

Recently, high-quality data were published on the algal growth inhibition caused by 50 non-polar narcotic compounds, of which 39 were liquid compounds with defined water solubility. In the present study, the toxicity data for these liquids were applied to challenge the chemical activity range for baseline toxicity. First, the reported effective concentrations (EC50) were divided by the respective water solubilities (Swater), since the obtained EC50/Swater ratio essentially equals the effective chemical activity (Ea50). The majority of EC50/Swater ratios were within the expected chemical activity range of 0.01–0.1 for baseline toxicity, and none of the ratios were significantly below 0.01. On a practical level, these findings suggest EC50 values for baseline toxicity to be at or above 1% of liquid solubility, which would have been accurate or conservative for all 39 liquids with defined water solubility in the applied dataset. On an environmental risk assessment level, predicted no-effect concentrations (PNECs) for baseline toxicity could even be set as a percentage of saturation, which can easily be extended to mixtures. However, EC50 values well below 1% of liquid saturation can still occur and would be a direct indication of excess toxicity.

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On the challenge to assess the exposure of organic contaminants in matrices with high partition coefficients

General information
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Passive dosing of pyrethroid insecticides to Daphnia magna: Expressing excess toxicity by chemical activity

Pyrethroid insecticides are nerve poisons and used as active ingredients in pesticide mixtures available for household and agriculture. The compounds are hydrophobic, and their strong sorption to organic material may result in decreasing exposure levels during toxicity tests and consequent underestimation of pyrethroid toxicity. This poster addresses three questions regarding the acute toxicity of pyrethroids towards the aquatic invertebrate Daphnia magna: (1) Is pyrethroid toxicity generally underestimated in the literature due to insufficiently controlled exposure levels? (2) At which chemical activity do pyrethroids exert their toxicity, and how similar are the effective chemical activities (Ea50) for different pyrethroids? (3) How much more toxic are pyrethroids relative to baseline toxicity? Toxicity experiments were conducted using passive dosing: Polydimethyl siloxane (PDMS) silicone was loaded with α-cypermethrin, esfenvalerate and bifenthrin, respectively, and then applied to control the exposure to D. magna for 48 h by equilibrium partitioning. In this way, the exposure was kept constant since various losses were efficiently buffered by re-partitioning from the polymer.

Based on results from the conducted passive dosing experiments and literature data, the three questions will be addressed in the following manner: (1) The effective concentration resulting in 50% immobilisation (EC50) will be determined for each of the three pyrethroids and compared to literature values, (2) Effective chemical activities resulting in 50% immobilisation (Ea50) will be estimated from pyrethroid EC50 values via the correlation of sub-cooled liquid solubility (S L, [mmol/L], representing a=1) and octanol to water partitioning ratios (Kow), (3) The excess toxicity observed for pyrethroids will be evaluated by comparing Ea50 values for individual pyrethroids to the chemical activity needed to initiate baseline toxicity (a=0.01-0.1).

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Copenhagen, University of California
Contributors: Nørgaard Schmidt, S., Gan, J., Kretschmann, A. C., Cedergreen, N., Mayer, P.
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Passive dosing to characterize the sorptive capacities of biota lipids from various trophic levels

General information
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Organisations: Department of Environmental Engineering, Environmental Chemistry, Stockholm University
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Relating Bioavailability Parameters to the Sorbent Characteristics of PAH Polluted Soils

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Sorptive capacities of lipids determined by passive dosing of non-polar organic chemicals

Lipids often are considered the major partitioning phase for non-polar organic chemicals. What is referred to as “lipid”, however, is a complex matrix consisting of a highly variable mixture of neutral (‘storage’) and polar (‘membrane’) lipids that usually is operationally defined by the extraction protocol. Furthermore, depending on an organism’s fraction of lipids and proteins and the properties of a chemical, other sorptive phases (e.g. proteins) may be particularly important. The aim of the present study was to expand our previous studies of the sorptive capacities of pure storage lipids into other pure phases and more realistic media, i.e. extractable organic matter (EOM) obtained by lipid extraction of various biota samples. Our experimental protocol included: i) extraction of biota tissues; ii) passive dosing of replicates of each EOM sample with cyclic volatile methylsiloxanes (cVMS), chlorobenzenes and polychlorinated biphenyls via a common headspace over an olive oil donor phase to transfer the same chemical activity into the samples; iii) sampling of EOM and olive oil controls at different time points; iv) purge-and-trap extraction of the model chemicals onto ENV+ SPE cartridges, elution and GC/MS analysis; v) characterization of the lipid composition in all samples via NMR. Our experiments demonstrate that the sorptive capacities of the EOM samples do not differ significantly from the olive oil controls if the EOM consists of neutral lipids only. However, the EOM samples show small but statistically significant differences in their sorptive capacities for the (semi)volatile model chemicals if other components such as phosphatidylcholine (PC) and cholesterol are present in quantifiable amounts. Based on the lipid composition quantified by NMR and literature data for
the chemicals’ partition ratios between PC/water and storage lipid/water, we modeled the chemicals’ partitioning into the EOM and compared the model results to the measured concentrations. The study provides a new basis for unravelling biomagnification, since an increase in concentration with trophic level can be divided into a sorption capacity effect and an increase in chemical activity.

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The Feasibility of Tree Coring as a Screening Tool for Selected Contaminants in the Subsurface

Chemical release resulting from inadequate care in the handling and storage of compounds has ultimately led to a large number of contaminated sites worldwide. Frequently found contaminants in the terrestrial environment include BTEX (benzene, toluene, ethylbenzene, and xylenes), heavy metals, PAHs (polycyclic aromatic hydrocarbons) and chlorinated solvents. The large number of contaminated sites has created a need for effective and reliable site investigations. In this PhD project the feasibility of tree coring as a screening tool for selected contaminants in the subsurface has been investigated to obtain more efficient site investigations. Trees have a natural ability to take up water and nutrients from the subsurface; consequently, contaminants can also enter the roots and be translocated to plant parts above ground where they will be absorbed, degraded or phytovolatilized depending on their physico-chemical properties. A small sample of the wood (a tree core) can be collected and analyzed to give information on potential subsurface contamination. To date the focus of tree coring has mainly been on the use as a screening tool for chlorinated solvents including perchloroethylene (PCE) and trichloroethylene (TCE), where the method has been applied with success. The results also showed that the measurements will be affected by various factors such as soil properties, climate conditions, sampling procedure, the tree species and especially the contaminants of interest.

The purpose of this PhD project is comprised of two primary objectives: (1) to investigate the feasibility of tree coring of different tree species as a screening tool for heavy metals, BTEX and PAHs in the subsurface and (2) to investigate under which conditions and for which purposes tree coring is a viable substitute for established site screening methods e.g. soil gas sampling. The first objective was achieved through tree core sampling campaigns from different tree species (e.g. willow, poplar, birch, cherry, and ash) at sites contaminated with heavy metals, BTEX or chlorinated solvents. The measured wood concentrations were compared to concentrations in soil, groundwater or soil gas. In addition, a laboratory study has been conducted to investigate the plant uptake of PAH from different soils. The second objective was accomplished by comparing wood concentrations attained through tree coring to measurements of soil gas, soil and/or groundwater attained through established site characterization methods. The site investigations showed that the use of tree coring as a screening tool for heavy metals and BTEX in the subsurface is more complex than for chlorinated solvents.

Heavy metals were expected to be good candidates for tree coring due to natural uptake mechanisms of essential heavy metals, but the use of tree coring to detect elevated heavy metal concentrations in soil is challenged by the presence of background concentrations. Therefore, a statistical comparison of the wood concentrations measured in trees grown at a potentially contaminated site and trees from a nearby non-contaminated site (reference trees) is necessary. This approach has demonstrated significantly elevated concentrations of zinc (Zn), copper (Cu), cadmium (Cd) and nickel (Ni) in trees grown at highly contaminated sites, while less or no significant elevated concentrations were found in trees from less contaminated sites. In addition, non-linear relationships were found between concentrations in wood and soil BTEX have similar physico-chemical properties as chlorinated solvents, so was expected that BTEX also would be good candidates for tree coring. However, the application of tree coring to locate BTEX-contaminated areas can be difficult as natural attenuation of the compounds (e.g. biodegradation and volatilization) may result in relatively low concentrations in the wood. Although difficult, investigations have shown that some BTEX contaminated areas can be detected by tree coring and that the concentrations of BTEX in wood can be correlated to those in soil gas, soil or groundwater. Precautions implemented to prevent cross-contamination have also shown to be important because it can otherwise lead to false positives. Among the sampled tree species, willows and poplars were the most suitable species for tree coring, since they were able to take up heavy metals and BTEX in highest concentrations. The laboratory study of PAH plant uptake from soil showed that the plant concentrations were not controlled by total soil concentrations or the bioavailable fraction in the soil. Concentrations measured in plant tissue above ground were more affected by deposition from air.

The comparison of tree coring and soil gas sampling for application as screening tools for chlorinated solvents showed that the two methods are complementary, which is why the choice of method to be used should be based on the specific purpose of the site investigation and the specific site conditions. In general, tree coring is a very rapid and low-invasive screening method, which provides an economic advantage to current methods. The low costs associated with tree coring allow for a high sampling density. This, together with a relatively large soil volume represented by a tree core, has shown to reduce the risk of overlooking contaminated areas and is a valuable method for the identification of previously unknown source areas within a short time period.
Transfer and effects of 1,2,3,5,7-pentachloronaphthalene in an experimental food chain

Polychlorinated naphthalenes are environmentally relevant compounds that are measured in biota at concentrations in the μg/kg lipid range. Despite their widespread occurrence, literature data on the accumulation and effects of these compounds in aquatic ecosystems are sparsely available. The goal of this study was to gain insights into the biomagnification and effects of 1,2,3,5,7-pentachloronaphthalene (PeCN52) in an experimental food chain consisting of benthic worms and juvenile rainbow trout. Worms were contaminated with PeCN52 by passive dosing from polydimethylsiloxane silicone. The contaminated worms were then used to feed the juvenile rainbow trout at 0.12, 0.25 or 0.50μg/gfish wet weight/day, and the resulting internal whole-body concentrations of the individual fish were linked to biological responses. A possible involvement of the cellular detoxification system was explored by measuring PeCN52-induced expression of the phase I biotransformation enzyme gene cyp1a1 and the ABC transporter gene abcb1a. At the end of the 28-day study, biomagnification factors were similar for all dietary intake levels with values between 0.5 and 0.7kg lipid fish/kg lipid worm. The average uptake efficiency of 60% indicated that a high amount of PeCN52 was transferred from the worms to the fish. Internal concentrations of up to 175mg/kg fish lipid in the highest treatment level did not result in effects on survival, behavior, or growth of the juvenile trout, but were associated with the induction of phase I metabolism which was evident from the significant up-regulation of cyp1a1 expression in the liver. In contrast, no changes were seen in abcb1a transcript levels.
Using a reference partitioning phase to link exposure and effect assessment of hydrophobic organic chemicals: Novel equilibrium partitioning concepts and methods

General information
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Using equilibrium passive dosing to maintain stable exposure concentrations of triclosan in a 6-week toxicity test

Aquatic organisms are constantly exposed to hydrophobic organic contaminants. Although these chemicals may be present at low concentrations, they can still cause negative long-term effects on organisms. In chemicals risk assessment, the majority of the ecotoxicological data is based on acute toxicity tests. Yet, the European Commission’s criteria for chemicals’ risk assessments aim at protecting higher levels in the environment. To achieve protection of populations and ecosystems, reliable long-term ecotoxicological tests are needed. In this study, we used equilibrium passive dosing to maintain stable exposure concentrations of triclosan (log Kow 4.8) in a 6-week multigeneration test with the benthic copepod Nitocra spinipes. The tests were performed in 10 mL vials casted with 1000 mg of silicone (DC 1-2577). Based on a previous pilot study, three triclosan concentrations were selected and tested (15 μg L-1; 30 μg L-1; 60 μg L-1) as well as a control (no triclosan). At test beginning, each vial contained 12 individuals consisting of 3 individuals from four different life stages. The test includes feeding with phytoplankton three times a week, which can lead to declining freely dissolved triclosan concentrations. In the present study this was buffered by passive dosing. Water was exchanged every 7th day by transferring the animals from the spend solution into a pre-equilibrated passive dosing glass. During the first two weeks, the copepods grow exponentially and can reach numbers of several hundred individuals in each vial. The increasing biomass of the test organisms can again lead to declining exposure concentrations, but such loss was buffered by passive dosing. Quality assurance tests showed that a) the loading and passive dosing procedures resulted in exposure concentrations with little variation (RSD 1-7 %), b) using two batches of passive dosing vials helped to maintain stable exposure concentrations, and c) the concentration of triclosan could be maintained throughout the whole 6-week test period. This study demonstrates that passive dosing offers a way forward to generate reliable and relevant toxicity data also from long-term studies with hydrophobic contaminants. The results on long-term toxicity of triclosan on Nitocra will be evaluated and discussed in relation to existing toxicity data from literature.

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Advancing passive sampling of contaminants in Environmental Science

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Research output: Research - peer-review Journal article – Annual report year: 2014
A novel passive dosing-based PICT detection method reveals no increased tolerance to benzene, toluene, ethylbenzene and xylene (BTEX) in soil bacterial communities exposed to gasoline vapours

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Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University, University of Copenhagen
Contributors: Modrzynski, J. J., Mayer, P., Christensen, J. H., Gilbert, D., Brandt, K.
Number of pages: 1
Publication date: 2014

Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries : Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:
A_novel_passive_dosing_based_PICT_detection_method_reveals_no_increased_tolerance_to_benzene_toluene_ethylbenzene_and_xylene_BTEX_in_soil_bacterial_communities_exposed_to_gasoline_vapours.pdf

Bibliographical note
WE036
Research output: Research - peer-review → Conference abstract in proceedings – Annual report year: 2014

Chemical activity for integrated chemical assessment

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Toronto, Unilever, Aarhus University, Trent University
Contributors: Arnot, J., Mayer, P., Schmidt, S. N., Armitage, J. M., Gouin, T., McCarty, L., Mackay, D.
Pages: 397
Publication date: 2014

Host publication information
Title of host publication: Abstract book : SETAC North America 35th Annual Meeting
Place of publication: Vancouver, British Columbia
Publisher: Society of Environmental Toxicology and Chemistry
Article number: WP184 (Annual Meeting, Vol. 35).
Research output: Research - peer-review → Conference abstract in proceedings – Annual report year: 2014

Concerned about the T in PBT? Ask what fugacity and activity can do for you!

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Unilever, Trent University, Aarhus University, University of Toronto
Contributors: Mackay, D., Arnot, J., Gouin, T., Mayer, P., Schmidt, S. N., Armitage, J. M.
Pages: 398
Publication date: 2014

Host publication information
Title of host publication: Abstract book : SETAC North America 35th Annual Meeting
Place of publication: Vancouver, British Columbia
Publisher: Society of Environmental Toxicology and Chemistry
Article number: WP186 (Annual Meeting, Vol. 35).
Research output: Research - peer-review → Conference abstract in proceedings – Annual report year: 2014

Co-Transport of Polycyclic Aromatic Hydrocarbons by Motile Microorganisms Leads to Enhanced Mass Transfer under Diffusive Conditions.
The environmental chemodynamics of hydrophobic organic chemicals (HOCs) are often rate-limited by diffusion in stagnant boundary layers. This study investigated whether motile microorganisms can act as microbial carriers that
enhance mass transfer of HOCs through diffusive boundary layers. A new experimental system was developed that allows (1) generation of concentration gradients of HOCs under the microscope, (2) exposure and direct observation of microorganisms in such gradients, and (3) quantification of HOC mass transfer. Silicone O-rings were integrated into a Dunn chemotaxis chamber to serve as sink and source for polycyclic aromatic hydrocarbons (PAHs). This resulted in stable concentration gradients in water (>24 h). Adding the model organism Tetrahymena pyriformis to the experimental system enhanced PAH mass transfer up to hundred-fold (benzo[a]pyrene). Increasing mass transfer enhancement with hydrophobicity indicated PAH co-transport with the motile organisms. Fluorescence microscopy confirmed such transport. The effective diffusivity of T. pyriformis, determined by video imaging microscopy, was found to exceed molecular diffusivities of the PAHs up to four-fold. Cell-bound PAH fractions were determined to range from 28% (naphthalene) to 92% (pyrene). Motile microorganisms can therefore function as effective carriers for HOCs under diffusive conditions and might significantly enhance mobility and availability of HOCs.

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University
Contributors: Gilbert, D., Jakobsen, H. H., Winding, A., Mayer, P.
Number of pages: 7
Pages: 4368−4375
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Environmental Science & Technology (Washington)
Volume: 48
Issue number: 8
ISSN (Print): 0013-936X
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
Web of Science (2017): Impact factor 6.653
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
Web of Science (2016): Impact factor 6.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Web of Science (2015): Impact factor 5.393
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Web of Science (2012): Impact factor 5.257
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945
Web of Science (2011): Impact factor 5.228
Equilibrium Sampling to Determine the Thermodynamic Potential for Bioaccumulation of Persistent Organic Pollutants from Sediment

Equilibrium partitioning (EqP) theory is currently the most widely used approach for linking sediment pollution by persistent hydrophobic organic chemicals to bioaccumulation. Most applications of the EqP approach assume (I) a generic relationship between organic carbon-normalized chemical concentrations in sediments and lipid-normalized concentrations in biota and (II) that bioaccumulation does not induce levels exceeding those expected from equilibrium partitioning. Here, we demonstrate that assumption I can be obviated by equilibrating a silicone sampler with chemicals in sediment, measuring chemical concentrations in the silicone, and applying lipid/silicone partition ratios to yield concentrations in lipid at thermodynamic equilibrium with the sediment ($C_{\text{lip}} \leftrightarrow \text{Sed}$). Furthermore, we evaluated the validity of assumption II by comparing $C_{\text{lip}} \leftrightarrow \text{Sed}$ of selected persistent, bioaccumulative and toxic pollutants (polychlorinated biphenyls (PCBs) and hexachlorobenzene (HCB)) to lipid-normalized concentrations for a range of biota from a Swedish background lake. PCBs in duck mussels, roach, eel, pikeperch, perch and pike were mostly below the equilibrium partitioning level relative to the sediment, i.e., lipid-normalized concentrations were $\leq C_{\text{lip}} \leftrightarrow \text{Sed}$, whereas HCB was near equilibrium between biota and sediment. Equilibrium sampling allows straightforward, sensitive and precise measurement of $C_{\text{lip}} \leftrightarrow \text{Sed}$. We propose $C_{\text{lip}} \leftrightarrow \text{Sed}$ as a metric of the thermodynamic potential for bioaccumulation of persistent organic...
chemicals from sediment useful to prioritize management actions to remediate contaminated sites.

**General information**

State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Stockholm University, Swedish University of Agricultural Sciences
Contributors: Jahnke, A., MacLeod, M., Wickström, H., Mayer, P.
Number of pages: 8
Pages: 11352–11359
Publication date: 2014
Peer-reviewed: Yes

**Publication information**

Journal: Environmental Science and Technology
Volume: 48
Issue number: 19
ISSN (Print): 0013-936X

Ratings:

BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
Web of Science (2017): Impact factor 6.653
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
Web of Science (2016): Impact factor 6.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Web of Science (2015): Impact factor 5.393
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Web of Science (2012): Impact factor 5.257
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945
Web of Science (2011): Impact factor 5.228
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.979 SNIP 1.726
Web of Science (2010): Impact factor 4.827
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.86 SNIP 1.809
Impact of soil amendments and the plant rhizosphere on PAH behaviour in soil

Carbonaceous amendments reduce PAH dissolved concentrations (C_{free}), limiting their uptake and toxicity. A soil contaminated with PAHs was mixed with activated carbon (AC), charcoal or compost and planted with radish (Raphanus sativus L.), and C_{free}, chemical activities and diffusive uptake of the PAHs measured over 2 months. For AC, C_{free} and diffusive uptake were decreased by up to 94% compared to the unamended soil within one week. In addition, the sum chemical activity of the PAHs remained below the threshold for baseline toxicity. In contrast, charcoal and compost only led to modest reductions in C_{free} and diffusive uptake, with sum chemical activities that could potentially result in baseline toxicity being observed. Furthermore, both C_{free} and diffusive uptake were lower in the planted compared to unplanted soils. Therefore, only AC successfully reduced PAH acute toxicity in the soil, but plant-promoted microbial degradation may also play an important role in PAH attenuation.

General information
State: Published
Organisations: Department of Chemistry, CERE – Center for Energy Ressources Engineering, Department of Environmental Engineering, Environmental Chemistry, Universität des Saarlandes, Aarhus University
Contributors: Marchal, G., Smith, K. E., Mayer, P., Wollesen de Jonge, L., Karlson, U. G.
Pages: 124-131
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Environmental Pollution
Volume: 188
ISSN (Print): 0269-7491
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5 SJR 1.615 SNIP 1.46
Web of Science (2017): Impact factor 4.358
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.27 SJR 1.827 SNIP 1.74
Web of Science (2016): Impact factor 5.099
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.72 SJR 2.003 SNIP 1.75
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.57 SJR 1.987 SNIP 2.005
Web of Science (2014): Impact factor 4.143
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.35 SJR 1.976 SNIP 1.94
Web of Science (2013): Impact factor 3.902
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 4.03 SJR 2.038 SNIP 1.74
Web of Science (2012): Impact factor 3.73
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.87 SJR 2.041 SNIP 1.745
Web of Science (2011): Impact factor 3.746
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.002 SNIP 1.64
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.002 SNIP 1.704
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.922 SNIP 1.718
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.843 SNIP 1.738
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.679 SNIP 1.799
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.51 SNIP 1.716
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.672 SNIP 1.675
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.562 SNIP 1.745
Scopus rating (2002): SJR 1.126 SNIP 1.421
Scopus rating (2001): SJR 1.142 SNIP 1.235
Scopus rating (2000): SJR 1.052 SNIP 1.06
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.028 SNIP 1
Original language: English
Is equilibrium sampling applicable in routine sediment monitoring?

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Goethe University Frankfurt
Contributors: Schaefer, S., Moehlenkamp, C., Claus, E., Heininger, P., Mayer, P.
Number of pages: 1
Publication date: 2014

Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries : Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:
Is_equilibrium_sampling_applicable_in_routine_sediment_monitoring.pdf

Bibliographical note
587
Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Juvenile swine evaluation of the ability of silicone rod in vitro digestors to predict PAH uptake across 20 different soils

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Saskatchewan
Contributors: Siciliano, S. D., James, K. J., Mayer, P.
Pages: 62-63
Publication date: 2014

Host publication information
Title of host publication: Abstract book : SETAC North America 35th Annual Meeting
Place of publication: Vancouver, British Columbia
Publisher: Society of Environmental Toxicology and Chemistry
Article number: 224
(Annual Meeting, Vol. 35).
Source: PublicationPreSubmission
Source-ID: 102162048
Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

PAH toxicity at aqueous solubility in the fish embryo test with Danio rerio using passive dosing

As part of the risk assessment process within REACh, prior to manufacturing and distribution of chemical substances their (eco)toxicological impacts have to be investigated. The fish embryo toxicity test (FET) with the zebrafish Danio rerio has gained a high significance as an in vitro alternative to animal testing in (eco)toxicology. However, for hydrophobic organic chemicals it remains a technical challenge to ensure constant freely dissolved concentration at the maximum exposure level during such biotests.

Passive dosing with PDMS silicone was thus applied to control the freely dissolved concentration of ten PAHs at their saturation level in the FET. The experiments gave repeatable results, with the toxicity of the PAHs generally increasing with the maximum chemical activities of the PAHs. HPLC analysis confirmed constant exposure at the saturation level. In additional experiments, fish embryos without direct contact to the silicone surface showed similar mortalities as those exposed with direct contact to the silicone. Silicone oil overlaying the water phase as a novel passive dosing phase had no observable effects on the development of the fish embryos until hatching.

This study provides further data to support the close relationship between the chemical activity and the toxicity of hydrophobic organic compounds. Passive dosing from PDMS silicone enabled reliable toxicity testing of (highly) hydrophobic substances at aqueous solubility, providing a practical way to control toxicity exactly at the maximum exposure level. This approach is therefore expected to be useful as a cost-effective initial screening of hydrophobic...
chemicals for potential adverse effects to freshwater vertebrates.

**General information**
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, RWTH Aachen University, Aarhus University, Saarland University, Heidelberg University
Number of pages: 8
Pages: 77-84
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: Chemosphere
Volume: 112
ISSN (Print): 0045-6535
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.62 SJR 1.435 SNIP 1.448
Web of Science (2017): Impact factor 4.427
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.39 SJR 1.447 SNIP 1.625
Web of Science (2016): Impact factor 4.208
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.04 SJR 1.497 SNIP 1.567
Web of Science (2015): Impact factor 3.698
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.76 SJR 1.59 SNIP 1.639
Web of Science (2014): Impact factor 3.34
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.92 SJR 1.721 SNIP 1.751
Web of Science (2013): Impact factor 3.499
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.5 SJR 1.794 SNIP 1.618
Web of Science (2012): Impact factor 3.137
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 3.61 SJR 1.962 SNIP 1.508
Web of Science (2011): Impact factor 3.206
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.879 SNIP 1.424
Web of Science (2010): Impact factor 3.155
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.842 SNIP 1.572
Partitioning of hydrophobic organic chemicals between silicone polymers and LDPE

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University, Hamburg University of Applied Sciences
Contributors: Gilbert, D., Witt, G., Smedes, F., Mayer, P.
Number of pages: 1
Publication date: 2014

Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries : Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:
Partitioning_of_hydrophobic_organic_chemicals_between_silicone_polymers_and_LDPE.pdf

Bibliographical note
TH052
Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Passive dosing as a tool to derive fugacity capacities of a variety of leaves for semi-volatile persistent organic contaminants

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Stockholm University
Contributors: Bolinius, D. J., Mayer, P., MacLeod, M., Mclachlan, M. S., Jahnke, A.
Number of pages: 1
Publication date: 2014
Passive dosing for the zebrafish embryo test using silicone O-rings

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Antwerp
Contributors: Vergauwen, L., Nørgaard Schmidt, S., Maho, W., Stickens, E., Hagenaars, A., Blust, R., Mayer, P., Covaci, A., Knapen, D.
Number of pages: 1
Publication date: 2014
Peer-reviewed: Yes
Event: Poster session presented at 3rd Symposium on Fish and Amphibian Embryos as Alternative Models in Teratology and Toxicology, Paris, France.

Electronic versions:
Poster.pdf
Source: PublicationPreSubmission
Source-ID: 104967476
Research output: Research - peer-review › Poster – Annual report year: 2015

Passive Equilibrium Sampling of Hydrophobic Organic Contaminants in Sediment

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Eastern Finland
Contributors: Jahnke, A., Maenpaa, K., Schaefer, S., Mayer, P.
Number of pages: 1
Publication date: 2014

Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries : Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:

Bibliographical note
TH065
Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Passive Equilibrium Sampling of Hydrophobic Organic Contaminants in Sediment

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Eastern Finland, Hamburg University of Applied Sciences, German Federal Institute of Hydrology (BfG)
Contributors: Jahnke, A., Mäenpää Joensuu, K., Witt, G., Schäfer, S., Mayer, P.
Number of pages: 1
Pages: 164
Publication date: 2014

Host publication information
Title of host publication: SETAC German Language Brange Annual Meeting: Abstract book
Article number: P35
Electronic versions:
Abstract book
Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Passive Equilibrium Sampling of Hydrophobic Organic Contaminants in Sediment

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Eastern Finland, Stockholm University, Hamburg University of Applied Sciences
Contributors: Jahnke, A., Maenpaa, K., Witt, G., Schaefer, S., Mayer, P.
Pages: 308
Publication date: 2014

Passive sampling methods for contaminated sediments: Scientific rationale supporting use of freely dissolved concentrations

Passive sampling methods (PSMs) allow the quantification of the freely dissolved concentration (C_{free}) of an organic contaminant even in complex matrices such as sediments. C_{free} is directly related to a contaminant's chemical activity, which drives spontaneous processes including diffusive uptake into benthic organisms and exchange with the overlying water column. Consequently, C_{free} provides a more relevant dose metric than total sediment concentration. Recent developments in PSMs have significantly improved our ability to reliably measure even very low levels of C_{free}.

Application of PSMs in sediments is preferably conducted in the equilibrium regime, where freely dissolved concentrations in the sediment are well-linked to the measured concentration in the sampler via analyte-specific partition ratios. The equilibrium condition can then be assured by measuring a time series or a single time point using passive samplers with different surface to volume ratios. Sampling in the kinetic regime is also possible and generally involves the application of performance reference compounds for the calibration. Based on previous research on hydrophobic organic contaminants, it is concluded that C_{free} allows a direct assessment of 1) contaminant exchange and equilibrium status between sediment and overlying water, 2) benthic bioaccumulation, and 3) potential toxicity to benthic organisms. Thus, the use of PSMs to measure C_{free} provides an improved basis for the mechanistic understanding of fate and transport processes in sediments and has the potential to significantly improve risk assessment and management of contaminated sediments.

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General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, ExxonMobil, Loyola Marymount University, University of California, Unilever, Massachusetts Institute of Technology, University of North Dakota, Ontario Ministry of the Environment, Hamburg University of Applied Sciences, Chinese Academy of Sciences, University of Queensland
Pages: 197-209
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Integrated Environmental Assessment and Management
Volume: 10
Issue number: 2
ISSN (Print): 1551-3777
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Passive sampling of polychlorinated biphenyls (PCB) in indoor air: towards a cost-effective screening tool
PCBs were widely used in construction materials in the 1960s and 1970s, a period of high building activity in Denmark. The objective of this study was therefore to use passive sampling techniques to develop a simple and cost-effective screening tool for PCBs in indoor air. The study proceeded in three phases combining a literature review, laboratory experiments and measurements in buildings potentially containing PCBs in indoor air. The laboratory experiments showed a strong influence of air velocity on the PCB partitioning between air and the passive sampler. Based on the results of the first two phases and comments from experts in the field of PCB containing construction materials, a kinetic sampler (petri dish with silicone) and a potential equilibrium sampler (silicone-coated paper) were tested in buildings. Calibration and validation were based on conventional active sampling, for both methods in their kinetic sampling phase. The methods were sensitive and precise, but tended to overestimate the concentration obtained by active sampling. More work will be needed to test the silicone-coated paper under equilibrium sampling conditions.

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University
Contributors: Vorkamp, K., Mayer, P.
Number of pages: 117
Publication date: 2014

Publication information
Physiological and molecular responses of springtails exposed to combined chemical and drought stress by passive dosing

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Aarhus University
Contributors: Schmidt, S. N., Holmstrup, M., Damgaard, C., Sørensen, J. G., Slotsbo, S., Mayer, P.
Number of pages: 1
Publication date: 2014

Host publication information
Title of host publication: Science Across Bridges, Borders and Boundaries : Programme Book
Place of publication: Basel, Switzerland
Publisher: SETAC-Europe
Electronic versions:
Physiological_and_molecular_responses_of_springtails_exposed_to_combined_chemical_and_drought_stress_by_passive_dosing.pdf

Bibliographical note
WE050
Research output: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

Physiological and molecular responses of springtails exposed to phenanthrene and drought
Interaction between effects of hazardous chemicals in the environment and adverse climatic conditions is a problem that receives increased attention in the light of climate change. We studied interactive effects of phenanthrene and drought using a test system in which springtails (Folsomia candida Willem) were concurrently exposed to a sublethal phenanthrene level via passive dosing from silicone (chemical activity of 0.010), and sublethal drought from aqueous NaCl solutions (water activity of 0.988). Previous studies have shown that the combined effects of high levels of phenanthrene and drought, respectively, interact synergistically when using lethality as an end-point. Here, we hypothesized that phenanthrene interferes with physiological mechanisms involved in drought tolerance, and that drought influences detoxification of phenanthrene. However, this hypothesis was not supported by data since phenanthrene had no effect on drought-protective accumulation of myo-inositol, and normal water conserving mechanisms of F. candida were functioning despite the near-lethal concentrations of the toxicant. Further, detoxifying induction of cytochrome P450 and glutathione-S-transferase was not impeded by drought. Both phenanthrene and drought induced transcription of heat shock protein (hsp70) and the combined effect of the two stressors on hsp70 transcription was additive, suggesting that the cellular stress and lethality imposed by these levels of phenanthrene and drought were also additive.

General information
State: Published
Organisations: Aarhus University
Contributors: Holmstrup, M., Slotsbo, S., Schmidt, S. N., Mayer, P., Damgaard, C., Sørensen, J. G.
Pages: 370-376
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Environmental Pollution
Volume: 184
ISSN (Print): 0269-7491
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5 SJR 1.615 SNIP 1.46
Web of Science (2017): Impact factor 4.358
Polyacrylate–water partitioning of biocidal compounds: Enhancing the understanding of biocide partitioning between render and water

In recent years, the application of polymer-based renders and paints for façade coatings of buildings has risen enormously due to the increased mounting of thermal insulation systems. These materials are commonly equipped with biocides - algaecides, fungicides, and bactericides - to protect the materials from biological deterioration. However, the biocides need to be present in the water phase in order to be active and, hence, they are flushed of the material by rain water. In order to increase the knowledge about the partitioning of biocides from render into the water phase, partition constants between the polymer - in this case polyacrylate - and water were studied using glass fibre filters coated with polyacrylate. The polyacrylate-water partition constants (logKAcW) of ten biocides used in construction material varied between 1.66 (isoproturon) and 3.57 (dichloro-N-octylisothiazolinone). The correlation of the polyacrylate-water partition constants with the octanol-water partition constants is significant, but the polyacrylate-water partition constants were predominantly below octanol-water partition constants (Kow). The comparison with render-water distribution constants showed that estimating the leaching of biocides from render based on polymer-water partitioning is a useful and practical tool.

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, University of Duisburg-Essen, Aarhus University
Contributors: Bollmann, U. E., Ou, Y., Mayer, P., Trapp, S., Bester, K.
Pages: 1021-1026
Publication date: 2014
Peer-reviewed: Yes
Silicone -Based Equilibrium Sampling of Sediment to Assess the Thermodynamic Potential of Trace-Level Hydrophobic Organic Contaminants to Bioaccumulate

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Swedish University of Agricultural Sciences, Stockholm University, Aarhus University
Contributors: Jahnke, A., MacLeod, M., Mclachlan, M., Wickström, H., Gilbert, D., Mayer, P.
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Silicone-Based Equilibrium Sampling of Sediment to Assess the Thermodynamic Potential of Trace-Level Hydrophobic Organic Contaminants to Bioaccumulate

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Silicone passive equilibrium samplers as 'chemometers' in eels and sediments of a Swedish lake.
Passive equilibrium samplers deployed in two or more media of a system and allowed to come to equilibrium can be viewed as 'chemometers' that reflect the difference in chemical activities of contaminants between the media. We applied silicone-based equilibrium samplers to measure relative chemical activities of seven 'indicator' polychlorinated biphenyls (PCBs) and hexachlorobenzene in eels and sediments from a Swedish lake. Chemical concentrations in eels and sediments were also measured using exhaustive extraction methods. Lipid-normalized concentrations in eels were higher than organic carbon-normalized concentrations in sediments, with biota–sediment accumulation factors (BSAFs) of five PCBs ranging from 2.7 to 12.7. In contrast, chemical activities of the same pollutants inferred by passive sampling were 3.5 to 31.3 times lower in eels than in sediments. The apparent contradiction between BSAFs and activity ratios is consistent with the sorptive capacity of lipids exceeding that of sediment organic carbon from this ecosystem by up to 50-fold. Factors that may contribute to the elevated activity in sediments are discussed, including slower response of sediments than water to reduced emissions, sediment diagenesis and sorption to phytoplankton. The 'chemometer' approach has the potential to become a powerful tool to study the thermodynamic controls on persistent organic chemicals in the environment and should be extended to other environmental compartments.

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Simultaneous Control of Phenanthrene and Drought by Dual Exposure System: The Degree of Synergistic Interactions in Springtails was Exposure Dependent

Organisms in the environment are exposed to multiple stressors. However, for terrestrial invertebrates, it remains difficult to study the effects of combined stressors under well-defined exposure conditions. Thus, the current study develops a new dual exposure system for the simultaneous and independent control of chemical and drought exposure in bioassays with terrestrial organisms: Passive dosing from silicone controlled the chemical activity of phenanthrene (chemical stress), while saline solutions controlled the water activity (drought stress) in the closed exposure system. The dual exposure system was then applied in a full factorial experiment with seven exposure levels ($7^2$), which aimed at determining the combined effects of phenanthrene and drought on the survival of the terrestrial springtail Folsomia candida after 7 d exposure. Fitting an "independent action" model to the complete data set revealed statistically significant synergy between phenanthrene and drought ($p < 0.0001$). However, the degree of synergy was exposure dependent with some synergy at higher and only minor synergy at lower exposure levels. This emphasizes the need for taking exposure levels into account when extrapolating synergy observations from (eco)toxicological studies done at high exposure levels.

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The effect of humic acids on biodegradation of polycyclic aromatic hydrocarbons depends on the exposure regime

Binding of polycyclic aromatic hydrocarbons (PAHs) to dissolved organic matter (DOM) can reduce the freely dissolved concentration, increase apparent solubility or enhance diffusive mass transfer. To study the effects of DOM on biodegradation, we used phenanthrene and pyrene as model PAHs, soil humic acids as model DOM and a soil Mycobacterium strain as a representative degrader organism. Humic acids enhanced the biodegradation of pyrene when present as solid crystals but not when initially dissolved or provided by partitioning from a polymer. Synchronous fluorescence spectrophotometry, scintillation counting and a microscale diffusion technique were applied in order to determine the kinetics of dissolution and diffusive mass transfer of pyrene. We suggest that humic acids can enhance or inhibit biodegradation as a result of the balance of two opposite effects, namely, solubilization of the chemicals on the one hand and inhibition of cell adhesion to the pollutant source on the other.

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Baseline Toxic Mixtures of Non-Toxic Chemicals: "Solubility Addition" Increases Exposure for Solid Hydrophobic Chemicals

This study addresses the question whether hydrophobic organic chemicals exerting no toxicity at their solubility limit (saturation) can form a toxic mixture. Spiking methods generally do not allow testing exactly at saturation without introducing micro-crystals. Passive dosing was thus applied to test the acute toxicity of several high melting point PAHs and their mixtures at the respective saturation levels to aquatic and terrestrial invertebrates. With the aquatic Daphnia magna, anthracene, chrysene, and benzo(a)pyrene resulted in no or limited acute toxicity (0-20%), whereas binary and tertiary mixtures of these resulted in significant acute toxicity (70-88%). Toxicity of PAHs and their mixtures could be fitted with one (sum) chemical activity-response curve in accordance with a similar mode of toxic action (i.e., concentration addition). The effective chemical activity (Ea-50) of 0.029 and the effective concentration on a lipid basis (EClipid, (eq).-50) of 95.7 mM were well within the range for baseline toxicity. Similar mixtures showed less toxicity to the terrestrial Folsomia candida due to steady-state body-burdens being below equilibrium partitioning levels. The results of the present study raise questions about the focus of risk assessment schemes and toxicity testing guidelines on individual substances, since apparently non-toxic chemicals might become toxic in a mixture.
Changes in Lumbriculus variegatus metabolites under hypoxic exposure to benzo(a)pyrene, chlorpyrifos and pentachlorophenol: Consequences on biotransformation

The regulation of endogenous metabolites is still not fully understood in aquatic invertebrates exposed concurrently to toxicants and hypoxia. Despite the prevalence of hypoxia in the aquatic environment, toxicity estimations seldom account for multiple stressors thereby differing from natural conditions. In this study, we examined the influence of hypoxia (<30%
O2) on contaminant uptake and the composition of intracellular metabolites in Lumbriculus variegatus exposed to benzo(a)pyrene (B(a)P, 3µg L(-1)), chloryrifos (CPF, 100µg L(-1)) or pentachlorophenol (PCP, 100µg L(-1)). Tissue extracts of worms were analyzed for 123 metabolites by gas chromatography-mass spectrometry and metabolite levels were then related to treatments and exposure time. Hypoxia markedly increased the accumulation of B(a)P and CPF, which underlines the significance of oxygen in chemical uptake. The oxygen effect on PCP uptake was less pronounced. Succinate and glycerol-3-phosphate increased significantly (p<0.0001) following hypoxic treatment, whereas sugars, cysteine, and cholesterol were effectively repressed. The buildup of succinate coupled with the corresponding decline in intracellular 2-oxo- and 2-hydroxy glutaric acid is indicative of an active hypoxia inducible factor mechanism. Glutamate, and TCA cycle intermediates (fumarate, and malate) were disturbed and evident in their marked suppression in worms exposed concurrently to hypoxia and PCP. Clearly, hypoxia was the dominant stressor for individuals exposed to B(a)P or CPF, but to a lesser extent upon PCP treatment. And since oxygen deprivation promotes the accumulation of different toxicants, there may be consequences on species composition of metabolites in natural conditions. Copyright 2013 Elsevier Ltd. All rights reserved.
Impact of soil amendments on the freely dissolved concentrations, chemical activities, and diffusive mass fluxes of PAHs in soil

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Is there sufficient ‘sink’ in current bioaccessibility determinations of organic pollutants in soils?
Bioaccessibility tests can be used to improve contaminated land risk assessments. For organic pollutants a ‘sink’ is required within these tests to better mimic their desorption under the physiological conditions prevailing in the intestinal tract, where a steep diffusion gradient for the removal of organic pollutants from the soil matrix would exist. This is currently ignored in most PBET systems. By combining the CEPBET bioaccessibility test with an infinite sink, the removal of PAH from spiked solutions was monitored. Less than 10% of spiked PAH remained in the stomach media after 1 h, 10% by 4 h in the small intestine compartment and c.15% after 16 h in the colon. The addition of the infinite sink increased bioaccessibility estimates for field soils by a factor of 1.2-2.8, confirming its importance for robust PBET tests. TOC or BC were not the only factors controlling desorption of the PAH from the soils. (C) 2013 Elsevier Ltd. All rights reserved.
Limited exposure originating from desorption resistant PAHs in soot

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Loss of artemisinin produced by Artemisia annua L. to the soil environment
Artemisia annua L synthesizes and accumulates the secondary metabolite artemisinin, a compound with antimalarial properties. As cultivation of the plant is still the only cost effective source of artemisinin, the production takes place in monocultures of A. annua. Artemisinin is known to have insecticidal and herbicidal effects, and also of being toxic to A. annua. Knowing the magnitude of the different routes of loss of artemisinin from A. annua to the soil environment makes it possible to reduce the risk of decrease in yield as well as reducing the impact on soil organisms including plants, and reducing the risk of leaching. The largest contributor (86-108%) of artemisinin loss to the soil environment was found to be from dead leaves. In the case with A. annua production, the risks can hence be limited by paying attention to the harvest and drying process, where risk of loss of plant material to the surrounding environment is the largest. Artemisinin is also lost from A. annua by rain runoff (<0.5%) and root excretion, but to a minor degree. The in situ silicone tube microextraction method was here successfully applied for the first time to monitor artemisinin from roots in an A. annua soil-plant system. (C) 2012 Elsevier B.V. All rights reserved.

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Methods to assess bioavailability of hydrophobic organic contaminants: Principles, operations, and limitations

Many important environmental contaminants are hydrophobic organic contaminants (HOCs), which include PCBs, PAHs, PBDEs, DDT and other chlorinated insecticides, among others. Owing to their strong hydrophobicity, HOCs have their final destination in soil or sediment, where their ecotoxicological effects are closely regulated by sorption and thus bioavailability. The last two decades have seen a dramatic increase in research efforts in developing and applying partitioning based methods and biomimetic extractions for measuring HOC bioavailability. However, the many variations of both analytical methods and associated measurement endpoints are often a source of confusion for users. In this review, we distinguish the most commonly used analytical approaches based on their measurement objectives, and illustrate their practical operational steps, strengths and limitations using simple flowcharts. This review may serve as guidance for new users on the selection and use of established methods, and a reference for experienced investigators to identify potential topics for further research. (C) 2012 Elsevier Ltd. All rights reserved.
A 7-day mixture toxicity experiment with the terrestrial springtail Folsomia candida was conducted, and the effects were linked to three different mixture exposure parameters. Passive dosing from silicone was applied to tightly control exposure levels and compositions of 12 mixture treatments, containing the polycyclic aromatic hydrocarbons (PAHs) naphthalene, phenanthrene, and pyrene. Springtail lethality was then linked to sum chemical activities (Sigma a), sum equilibrium lipid concentrations (Sigma C-lipid eq.), and sum toxic units (Sigma TU). In each case, the effects of all 12 mixture treatments could be fitted to one sigmoidal exposure response relationship. The effective lethal chemical activity (La50) of 0.027 was well within the expected range for baseline toxicity of 0.01-0.1. Linking the effects to the lipid based exposure parameter yielded an effective lethal concentration (Sigma C-lipid eq. 50) of 133 mmol kg(-1) lipid in good correspondence with the lethal membrane burden for baseline toxicity (40-160 mmol kg(-1) lipid). Finally, the effective lethal toxic unit (Sigma TU50) of 1.20 was rather close to the expected value of 1. Altogether, passive dosing provided tightly controlled mixture exposure in terms of both level and composition, while Sigma a, Sigma C-lipid eq., and Sigma TU allowed baseline toxicity to be linked to mixture exposure.
Passive Equilibrium Sampler for in Situ Measurements of Freely Dissolved Concentrations of Hydrophobic Organic Chemicals in Sediments

In this study, an equilibrium passive sampling device is introduced that facilitates the in situ measurement of hydrophobic organic chemicals bioavailability in sediments in terms of freely dissolved concentrations. The new field sampler allows SPME fibers and silicone hollow fibers to be immersed and equilibrated in situ, whereas an automated liner exchanger (ALEX) facilitates the quantitative transfer of analytes to the GC without the use of extraction solvents. The sampler was developed for environmental monitoring as follows: (1) It is of very solid construction and can be reused practically ad infinitum. (2) Fibers with varying surface to volume ratios can be exposed in parallel in order to confirm that equilibrium was reached between sampler and sediment. (3) The equilibrium times allow a temporal resolution that is suited for monitoring of both long-term trends and seasonal effects. The automated thermal desorption reduced sample treatment to a minimum and ensured cost- and time-efficient measurements while minimizing potential error sources after the sampling. The sampler is applicable in a multitude of aquatic environments, especially where currents are low and sediments are muddy and well-mixed, e.g. by bioturbation. Examples for such environments are mud flats, harbor basins, river banks, and lakes.

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Sorptive Bioaccessibility Extraction (SBE) of soils - combining mobilisation medium with absorption sink

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Sorptive Physiologically Based Extraction of Contaminated Solid Matrices: Incorporating Silicone Rod As Absorption Sink for Hydrophobic Organic Contaminants

The oral bioaccessibility of soil contaminants is increasingly assessed with physiologically based extraction tests (PBETs): the contaminant fraction that is desorbed into simulated digestive fluids is measured and classified as bioaccessible. However, this approach can lead to underestimations if the capacity of the fluids is insufficient to provide infinite sink conditions. Desorption will then progressively decrease and finally stop when equilibrium between soil and medium is reached. To circumvent this artifact, we incorporated a silicone rod as an absorption sink into the PBET to continuously absorb mobilized contaminants and maintain the desorption gradient. Polycyclic aromatic hydrocarbons served as model contaminants and the colon extended PBET as the extraction model. The inclusion of the silicone rod sink (1) increased the extraction capacity of the test by orders of magnitude, (2) ensured near infinite sink conditions, and (3) allowed for simple back-extraction of PAHs for their quantification by GC-MS. The silicone rod provided fast enrichment when applied to the stomach and small intestine compartment, but was somewhat slower in the richer colon compartment. Finally, the sorptive-PBET was applied to wood soot and a kindergarten soil. The present article provides the basis for how an absorption sink can be integrated into PBET models.

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The dosing determines mutagenicity of hydrophobic compounds in the Ames II assay with metabolic transformation: Passive dosing versus solvent spiking

The Ames II bacterial mutagenicity assay is a new version of the standard Ames test for screening chemicals for genotoxic activity. However, the use of plastic micro-titer plates has drawbacks in the case of testing hydrophobic mutagens, since sorptive and other losses make it difficult to control and define the exposure concentrations, and they reduce availability for bacterial uptake or to the S9 enzymes. With passive dosing, a biocompatible polymer such as silicone is loaded with the test compound and acts as a partitioning source. It compensates for any losses and results in stable freely dissolved concentrations. Passive dosing using silicone O-rings was applied in the Ames II assay to measure PAH mutagenicity in strains TA98 and TAMix - a mixture of six different bacterial strains detecting six different base-pair substitutions - after metabolic activation by S9. Initially, 10 PAHs were tested with passive dosing from saturated O-rings, aiming at levels in the test medium close to aqueous solubility. Fluoranthene, pyrene and benzo(a)pyrene were mutagenic in both TA98 and TAMix, whereas benz(a)anthracene was mutagenic in TA98 only. The concentration-dependent mutagenic activity of benzo(a)pyrene was then compared for passive dosing and solvent spiking. With spiking, nominal concentrations greatly exceeded aqueous solubility before mutagenicity was observed, due to sorptive losses and limiting dissolution kinetics. In contrast, the passive dosing concentration-response curves were more reproducible, and shifted towards lower concentrations by several orders of magnitude. This study raises fundamental questions about how to introduce hydrophobic test substances in the Ames II assay with biotransformation, since the measured mutagenicity not only depends on the compound potency but also on its supply, sorption and consumption during the assay. (C) 2012 Elsevier B.V. All rights reserved.
Uptake and toxicity of polycyclic aromatic hydrocarbons in terrestrial springtails-studying bioconcentration kinetics and linking toxicity to chemical activity

Passive dosing applies a polymer loaded with test compound(s) to establish and maintain constant exposure in laboratory experiments. Passive dosing with the silicone poly(dimethylsiloxane) was used to control exposure of the terrestrial springtail Folsomia candida to six polycyclic aromatic hydrocarbons (PAHs) in bioconcentration and toxicity experiments. Folsomia candida could move freely on the PAH-loaded silicone, resulting in exposure via air and direct contact. The bioconcentration kinetics indicated efficient uptake of naphthalene, anthracene, and pyrene through air and (near) equilibrium partitioning of these PAHs to lipids and possibly the waxy layer of the springtail cuticle. Toxicities of naphthalene, phenanthrene, and pyrene were related to chemical activity, which quantifies the energetic level and drives spontaneous processes including diffusive biouptake. Chemical activityresponse relationships yielded effective lethal chemical activities (La50s) well within the expected range for baseline toxicity (0.010.1). Effective lethal body burdens for naphthalene and pyrene exceeded the expected range of 2 to 8 mmol kg-1 fresh weight, which again indicated the waxy layer to be a sorbing phase. Finally, chemical activities were converted into equilibrium partitioning concentrations in lipids yielding effective lethal concentrations for naphthalene and phenanthrene in good correspondence with the lethal membrane burden for baseline toxicity (40160?mmol kg-1 lipid). Passive dosing was a practical approach for tightly controlling PAH exposure, which in turn provided new experimental possibilities and findings. Environ. Toxicol. Chem. 2013;32:361369. (C) 2012 SETAC
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Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.534 SNIP 1.184
Web of Science (2005): Indexed yes
A flow-through passive dosing system for continuously supplying aqueous solutions of hydrophobic chemicals to bioconcentration and aquatic toxicity tests

A continuous supply of water with defined stable concentrations of hydrophobic chemicals is a requirement in a range of laboratory tests such as the OECD 305 protocol for determining the bioconcentration factor in fish. Satisfying this requirement continues to be a challenge, particularly for hydrophobic chemicals. Here we present a novel solution based on equilibrium passive dosing. It employs a commercially available unit consisting of similar to 16000 polydimethylsiloxane (PDMS) tubes connected to two manifolds. The chemicals are loaded into the unit by repeatedly perfusing it with a methanol solution of the substances that is progressively diluted with water. Thereafter the unit is perfused with water and the chemicals partition from the unit into the water. The system was tested with nine chemicals with logK(ow) ranging from 4.1 to 6.3. The aqueous concentrations generated were shown to be largely independent of the water flow rate, and the unit to unit reproducibility was within a factor of similar to 2. In continuous flow experiments the aqueous concentrations of most of the study chemicals remained constant over 8 d. A model was assembled that allows prediction of the operating characteristics of the system from the logKow or PDMS/water partition coefficient of the chemical. The system is a simple, safe, predictable and flexible tool that generates stable aqueous concentrations of hydrophobic chemicals. (C) 2011 Elsevier Ltd. All rights reserved.
Contaminant trap - Isolating and measuring the desorption resistant pool of soil pollutants

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Contributors: Mayer, P.
Pages: 76-78
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Host publication information
Title of host publication: Model-Driven Soil Probing, Site Assessment and Evaluation Guidance on Technologies
Publisher: Sapienza Universitá Editrice
Editors: Kästner, M., Braeckevelt, M., Döberl, G., Cassiani, G., Petrangeli Papini, M., Leven-Pfister, C., van Ree, D.
ISBN (Print): 978-88-95814-72-8
Source: PXA Import
Source-ID: 51880903
Research output: Research - peer-review > Book chapter – Annual report year: 2013

Dynamic Passive Dosing for Studying the Biotransformation of Hydrophobic Organic Chemicals: Microbial Degradation as an Example
Biotransformation plays a key role in hydrophobic organic compound (HOC) fate, and understanding kinetics as a function of (bio)availability is critical for elucidating persistence, accumulation, and toxicity. Biotransformation mainly occurs in an aqueous environment, posing technical challenges for producing kinetic data because of low HOC solubilities and sorptive losses. To overcome these, a new experimental approach based on passive dosing is presented. This avoids using cosolvent for introducing the HOC substrate, buffers substrate depletion so biotransformation is measured within a narrow and defined dissolved concentration range, and enables high compound turnover even at low concentrations to simplify end point measurement. As a case study, the biodegradation kinetics of two model HOCs by the bacterium Sphingomonas paucimobilis EPA505 were measured at defined dissolved concentrations ranging over 4 orders of magnitude, from 0.017 to 658 μg L−1 for phenanthrene and from 0.006 to 90.0 μg L−1 for fluoranthene. Both compounds had similar mineralization fluxes, and these increased by 2 orders of magnitude with increasing dissolved concentrations. First-order mineralization rate constants were also similar for both PAHs, but decreased by around 2 orders of magnitude with increasing dissolved concentrations. Dynamic passive dosing is a useful tool for measuring biotransformation kinetics at realistically low and defined dissolved HOC concentrations.

General information
State: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering, Aarhus University
Contributors: Smith, K. E. C., Rein, A., Trapp, S., Mayer, P.; Karlson, U. G.
Pages: 4852-4860
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Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
Web of Science (2017): Impact factor 6.653
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
Web of Science (2016): Impact factor 6.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Equilibrium sampling of organic soil pollutants

General information
State: Published
Organisations: Aarhus University
Contributors: Mayer, P.
Pages: 79-81
Publication date: 2012

Host publication information
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Editors: Kästner, M., Braeckevelt, M., Döberl, G., Cassiani, G., Petrangeli Papini, M., Leven-Pfister, C., van Ree, D.
ISBN (Print): 978-88-95814-72-8
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Research output: Research › Book chapter – Annual report year: 2013

Long-Term Effects of Legacy Copper Contamination on Microbial Activity and Soil Physical Properties
Soils heavily contaminated with copper (Cu) are considered unsuitable for agricultural use due to adverse impacts on microbial activity, soil physical properties, and direct toxicity to crops. This study investigated effects of Cu pollution from timber preservation activities between 1911 and 1924 on soil micro-organisms and subsequent effects on physical properties of a sandy loam soil. Tillage operations over the last 70 years have caused spreading of the initially localized contamination and have created a Cu concentration gradient from 20 to 3800 mg kg⁻¹ across an agricultural field in Hygum, Denmark. Soil samples obtained from the fallow field were used to determine total microbial activity using fluorescein diacetate and dehydrogenase assays. The physical properties measured included water-dispersible clay, bulk density, air permeability and air-filled porosity. Significant differences in microbial activity (for both assays) were observed at Cu concentrations >500 mg kg⁻¹. Although, unfavorable changes in all physical properties were obvious for Cu concentrations >500 mg kg⁻¹, significant increases in bulk density and water dispersible-clay, together with decreases in total porosity, air-filled porosity and air permeability occurred for Cu concentrations >900 mg kg⁻¹. There was significant negative correlation between microbial activity and the susceptibility of clay dispersion by water. These results suggest that a threshold level for Cu exists (~500 mg kg⁻¹ for this soil type) beyond which microbial activity decreases and soil structure becomes more compact with reduced permeability to air and water.

Measuring binding and speciation of hydrophobic organic chemicals at controlled freely dissolved concentrations and without phase separation
The binding and speciation of hydrophobic organic chemicals (HOCs) in aqueous solutions were determined by controlling chemical activity and measuring total concentrations. Passive dosing was applied to control chemical activities of HOCs in aqueous solutions by equilibrium partitioning from a poly(dimethylsiloxane) polymer preloaded with the chemicals. The HOC concentrations in the equilibrated solutions [C-solution(eq)] and water [C-water(eq)] were then measured. Free fractions of the HOCs were determined as C-water(eq)/C-solution(eq), whereas enhanced capacities (E) of the solutions for HOCs were determined as C-solution(eq)/C-water(eq). A mixture of polycyclic aromatic hydrocarbons served as model analytes, while humic acid, sodium dodecyl sulfate, hydroxypropyl-beta-cyclodextrin, and NaCl served as model medium constituents. The enhanced capacities were plotted versus the concentrations of medium constituents, and simple linear regression provided precise partition ratios, salting out constants, and critical micelle concentrations. These parameters were generally in good agreement with published values obtained by solid phase microextraction and fluorescence quenching. The very good precision was indicated by the low relative standard errors for the partition ratios of 0.5-8%,
equivalent to 0.002-0.03 log unit. This passive dosing approach allows binding and speciation of HOCs to be studied without any phase separation steps or mass balance assumptions.
Partitioning of fluoranthene between free and bound forms in stormwater runoff and other urban discharges using passive dosing

Partitioning of fluoranthene in stormwater runoff and other urban discharges was measured by a new analytical method based on passive dosing. Samples were collected at the inlet (n = 11) and outlet (n = 8) from a stormwater retention pond in Albertslund (Denmark), and for comparison samples were also obtained at a municipal wastewater treatment plant, a power plant, a contaminated site and a waste deposit in Copenhagen (n = 1 at each site). The freely dissolved concentration of 14C-fluoranthene in the samples was controlled by equilibrium partitioning from a pre-loaded polymer and the total sample concentration measured. The measurements yielded free fractions of fluoranthene in stormwater in the range 0.04–0.15 in the inlet during the first part of the runoff events increasing to 0.3–0.5 at the end of the events and in the outlet from the retention pond. The enhanced capacity of the different stormwater samples for carrying fluoranthene was 2–23 relative to pure water and decreasing during rain events. The enhanced capacity of stormwater showed a different relationship with suspended solid concentrations than the other types of urban discharges. Partitioning of fluoranthene to dissolved organic carbon was lower than partitioning to particulate organic carbon. Partitioning of fluoranthene to particulate organic matter in the 19 stormwater samples yielded a log KPOM of 5.18. The presented results can be used in stormwater quality modeling and assessment of efficiency of stormwater treatment systems. This work also shows the potential of the passive dosing method to obtain conversion factors between total concentrations, which are needed for comparison with water quality criteria, and freely dissolved concentrations, which are more related to toxicity and obtained by the use of most passive samplers.

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering
Contributors: Birch, H., Mayer, P., Lützhøft, H. H., Mikkelsen, P. S.
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Journal: Water Research
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Web of Science (2018): Indexed yes
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Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.358
Web of Science (2017): Impact factor 7.051
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.49 SJR 2.663 SNIP 2.563
Web of Science (2016): Impact factor 6.942
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.63 SJR 2.665 SNIP 2.482
Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Pulmonary Surfactant Suppressed Phenanthrene Adsorption on Carbon Nanotubes through Solubilization and Competition As Examined by Passive Dosing Technique

Adsorption of phenanthrene on carbon nanotubes (CNTs) was examined in the presence of pulmonary surfactant (Curosurf) and its main components, dipalmitoyl phosphatidylcholine (DPPC) and bovine serum albumin (BSA). A passive-dosing method based on equilibrium partitioning from a preloaded polymer was successfully employed to measure phenanthrene binding and speciation at controlled freely dissolved concentrations while avoiding phase separation steps. Curosurf, DPPC, and BSA could all linearly solubilize phenanthrene, and phenanthrene solubilization by Curosurf was 4 times higher than individual components (DPPC or BSA). In the presence of Curosurf, DPPC or BSA, adsorption of phenanthrene by multiwalled CNTs (MWCNTs) was suppressed, showing competitive adsorption between pulmonary surfactant (or DPPC, BSA) and phenanthrene. Competitive adsorption between Curosurf and phenanthrene was the strongest. Therefore, when phenanthrene-adsorbed CNTs enter the respiratory tract, phenanthrene can be desorbed due to both solubilization and competition. The bioaccessibility of phenanthrene adsorbed on three MWCNTs in the respiratory tract would be positively related to the size of their outer diameters. Moreover, the contribution of solubilization and competition to desorption of phenanthrene from MWCNTs was successfully separated for the first time. These findings demonstrate the two mechanisms on how pulmonary surfactants can enhance desorption and thus possibly biological absorption of phenanthrene adsorbed on CNTs.

General information
State: Published
Organisations: Ocean University of China, University of Massachusetts, Hebrew University of Jerusalem, Aarhus University
Contributors: Zhao, J., Wang, Z., Mashayekhi, H., Mayer, P., Chefetz, B., Xing, B.
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Publication date: 2012
Peer-reviewed: Yes

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Issue number: 10
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  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 2
  Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
  Web of Science (2017): Impact factor 6.653
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
  Web of Science (2016): Impact factor 6.198
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
  Web of Science (2015): Impact factor 5.393
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
  Web of Science (2014): Impact factor 5.33
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
  Web of Science (2013): Impact factor 5.481
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 2
  Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
  Web of Science (2012): Impact factor 5.257
  ISI indexed (2012): ISI indexed yes
The toxicity testing of hydrophobic organic compounds (HOCs) in aquatic media is generally challenging, and this is even more problematic for mixtures. The hydrophobic properties of these compounds make them difficult to dissolve, and subsequently to maintain constant exposure concentrations. Evaporative and sorptive losses are highly compound-specific, which can alter not only total concentrations, but also, the proportions between the compounds in the mixture. Therefore, the general aim of this study was to explore the potential of passive dosing for testing the toxicity of a PAH mixture that recreates the mixture composition found in seawater from a coastal area of Spain, the Bay of Algeciras. First, solvent spiking and passive dosing were compared for their suitability to determine the acute toxicity to Artemia franciscana nauplii of several PAHs at their respective solubility limits. Second, passive dosing was applied to recreate the seawater mixture composition of PAHs measured in a Spanish monitoring program, to test the toxicity of this mixture at different levels. HPLC analysis was used to confirm the reproducibility of the dissolved exposure concentrations for the individual PAHs and mixtures. This study shows that passive dosing has some important benefits in comparison with solvent spiking for testing HOCs in aquatic media. These include maintaining constant exposure concentrations, leading to higher reproducibility and a relative increase in toxicity. Passive dosing is also able to faithfully reproduce real mixtures of HOCs such as PAHs, in toxicity tests, reproducing both the levels and proportions of the different compounds. This provides a useful approach for studying the toxicity of environmental mixtures of HOCs, both with a view to investigating their toxicity but also for determining safety factors before such mixtures result in detrimental effects. (C) 2012 Elsevier B.V. All rights reserved.
Sensitive Equilibrium Sampling To Study Polychlorinated Biphenyl Disposition in Baltic Sea Sediment

An equilibrium sampling approach using glass jars with pm thin coatings of the silicone polydimethylsiloxane (PDMS) was validated and applied to background sediment samples from a >50 km transect in the Stockholm Archipelago. Equilibrium between the sediment and the PDMS was demonstrated using different coating thicknesses. From the concentrations of polychlorinated biphenyls (PCBs) in the PDMS, we assessed (i) freely dissolved concentrations in the sediment interstitial porewater (C-Sediment_free); (ii) the equilibrium bromium status between sediment and water; (iii) the equilibrium status between sediment and biota; and (iv) site-specific sediment/water distribution ratios (K-D). The results showed that (i) Stockholm was a source of PCBs to the Baltic Sea as evidenced by significantly higher C-Sediment_free in Stockholm Harbor; (ii) the fugacity in sediment exceeded that in water (monitoring samples collected in February) by an average factor of 4.0; (iii) the fugacity in sediment exceeded that in herring by an average factor of 5.2; and (iv) K-D near Stockholm Harbor was 0.3-1.7 log units greater than in the outer archipelago. The coated glass jar method with its high precision and built-in QA/QC opens new possibilities to study the disposition of hydrophobic chemicals at trace levels (C-Sediment_free down to 1.06 fg/L) in background environments.
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Web of Science (2015): Impact factor 5.393
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Web of Science (2012): Impact factor 5.257
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945
Web of Science (2011): Impact factor 5.228
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.979 SNIP 1.726
Web of Science (2010): Impact factor 4.827
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.86 SNIP 1.809
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.96 SNIP 1.935
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.774 SNIP 1.914
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.55 SNIP 1.893
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.608 SNIP 1.999
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.86 SNIP 2.046
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.54 SNIP 2.065
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.392 SNIP 1.949
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.387 SNIP 1.968
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 3.03 SNIP 2.315
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 3.367 SNIP 2.351

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DOIs:
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Research output: Research - peer-review › Journal article – Annual report year: 2013
Soil microbial and physical properties and their relations along a steep copper gradient
Copper (Cu) is accumulating in agricultural soils because it is an essential component of mineral fertilizers and pesticides. This could lead to toxic effects on soil macro- and micro-organisms and impact soil structure development. We investigated the effect of historical Cu contamination (>80 years; from background concentrations up to 3837 mg Cu kg\(^{-1}\)) on soil microbial enzyme activity, physical properties and resilience to compression. Soil samples and cores were taken from a fallow sandy loam field in Denmark. Microbial activity was quantified using fluorescein diacetate (FDA) and dehydrogenase (DHA) assays. Water dispersible clay was measured on field moist and air dried samples. For the resilience assay, soil cores (drained to -100 hPa) were subjected to uniaxial confined compression (200 kPa) followed by wet-dry or freeze-thaw cycles. Microbial enzyme activity significantly decreased with Cu concentration greater than or similar to 500 mg kg\(^{-1}\) with the two microbial assays linearly correlated with each other as well as with the water dispersible clay. An effect concentration causing a 50% reduction (EC50) in enzyme activity was observed at 521 mg kg\(^{-1}\) for FDA and 542 mg kg\(^{-1}\) for DHA. Significant increases in water dispersible clay, bulk density and decreases in air-filled porosity and air permeability were observed from Cu greater than or similar to 900 mg kg\(^{-1}\). The increased density of the contaminated soils led to greater compression resistance and resilience relative to the uncontaminated soil. The results suggest that a threshold level for Cu exists (similar to 500 mg kg\(^{-1}\) for this soil type) beyond which microbial activity decreases and soil structure becomes more compact with reduced permeability to air. (C) 2012 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Aarhus University, Aalborg University
Contributors: Arthur, E., Moldrup, P., Holmstrup, M., Schjønning, P., Winding, A., Mayer, P., de Jonge, L. W.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.32
Web of Science (2017): Impact factor 2.916
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.41
Web of Science (2016): Impact factor 2.786
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.99
Web of Science (2015): Impact factor 2.67
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.89
Web of Science (2014): Impact factor 2.644
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.7
Web of Science (2013): Impact factor 2.206
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.32
Web of Science (2012): Impact factor 2.106
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Sorptive Bioaccessibility Extraction (SBE) of Soils: Combining a Mobilization Medium with an Absorption Sink

In principle, soil bioaccessibility extraction methods are simple dissolution experiments, where the fraction of compounds that is transferred to the extraction medium is measured and considered to be bioaccessible. For hydrophobic organic chemicals (HOCs) such techniques can lead to underestimation of bioaccessibility when the capacity of the extraction medium is insufficient to provide infinite sink conditions for the target compounds. A sorptive bioaccessibility extraction (SBE) method was thus developed and validated, which integrates the key processes of desorption from the matrix and subsequent consumption or depletion. Cyclodextrin was used as a diffusive carrier to enhance desorption from the matrix, while a silicone rod was used as a dominating sink that continuously absorbed the HOC molecules from the cyclodextrin solution. The silicone rod was then solvent extracted and the HOCs measured by GC-MS. For wood soot, the SBE method yielded PAH bioaccessibility estimates that were 3-24 times higher compared to a cyclodextrin extraction without a sink. The study demonstrated that the inclusion of an absorption sink into an established bioaccessibility extraction method (1) is rather simple, (2) can have a major impact on the obtained results, especially for the more hydrophobic compounds and (3) can simplify the analytics.

General information
State: Published
Organisations: Aarhus University
Contributors: Gouliarmou, V., Mayer, P.
Pages: 10682-10689
Publication date: 2012
Peer-reviewed: Yes

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Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
Web of Science (2017): Impact factor 6.653
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
Web of Science (2016): Impact factor 6.198
Web of Science (2016): Indexed yes
Speciation of PAHs in stormwater

General information
State: Published
Organisations: Department of Environmental Engineering, Urban Water Engineering
Contributors: Birch, H., Mayer, P., Lützhøft, H. H., Mikkelsen, P. S.
Number of pages: 1
Pages: 153
Publication date: 2012

Host publication information
Title of host publication: Abstract Book : 6th SETAC World Congress/SETAC Europe 22nd Annual Meeting
Publisher: Society of Environmental Toxicology and Chemistry
Electronic versions: prod21341903121293.Abstractbook1_Part2.pdf
URLs: http://berlin.setac.eu/scientific_programme/download_the_abstracts_book/?contentid=582&pr_id=403&last=435

Bibliographical note
Abstract: MO 035

Time-Weighted Average SPME Analysis for in Planta Determination of cVOCs
The potential of phytoscreening for plume delineation at contaminated sites has promoted interest in innovative, sensitive contaminant sampling techniques. Solid-phase microextraction (SPME) methods have been developed, offering quick, undemanding, noninvasive sampling without the use of solvents. In this study, time-weighted average SPME (TWA-SPME) sampling was evaluated for in planta quantification of chlorinated solvents. TWA-SPME was found to have increased sensitivity over headspace and equilibrium SPME sampling. Using a variety of chlorinated solvents and a polydimethylsiloxane/carboxen (PDMS/CAR) SPME fiber, most compounds exhibited near linear or linear uptake over the sampling period. Smaller, less hydrophobic compounds exhibited more nonlinearity than larger, more hydrophobic molecules. Using a specifically designed in planta sampler, field sampling was conducted at a site contaminated with chlorinated solvents. Sampling with TWA-SPME produced instrument responses ranging from 5 to over 200 times higher than headspace tree core sampling. This work demonstrates that TWA-SPME can be used for in planta detection of a broad range of chlorinated solvents and methods can likely be applied to other volatile and semivolatile organic compounds.

General information
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Organisations: Missouri University of Science and Technology, Aarhus University
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
Web of Science (2017): Impact factor 6.653
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
Web of Science (2016): Impact factor 6.198
Web of Science (2016): Indexed yes
Towards a renewed research agenda in ecotoxicology

New concerns about biodiversity, ecosystem services and human health triggered several new regulations increasing the need for sound ecotoxicological risk assessment. The PEER network aims to share its view on the research issues that this challenges. PEER scientists call for an improved biologically relevant exposure assessment. They promote comprehensive effect assessment at several biological levels. Biological traits should be used for Environmental risk assessment (ERA) as promising tools to better understand relationships between structure and functioning of ecosystems. The use of modern high throughput methods could also enhance the amount of data for a better risk assessment. Improved models coping with multiple stressors or biological levels are necessary to answer for a more scientifically based risk assessment. Those methods must be embedded within life cycle analysis or economical models for efficient regulations. Joint research programmes involving humanities with ecological sciences should be developed for a sound risk management. (C) 2011 Elsevier Ltd. All rights reserved.
Application of passive dosing to study the biotransformation and biodegradation of hydrophobic

**General information**
- State: Published
- Organisations: Department of Environmental Engineering, KWR Water Cycle Research Institute, Danish Centre for Environment and Energy
- Contributors: Smith, K. E. C., Rein, A., Heringa, M., Mayer, P., Gosewinkel, U. B.
- Publication date: 15 May 2011
- Peer-reviewed: No
- Source: PXA Import
- Source-ID: 37368172
- Research output: Research - peer-review › Journal article – Annual report year: 2013

**DoIs:**
10.1016/j.envpol.2011.08.011

Calibrating passive sampling and passive dosing techniques to lipid based concentrations

**General information**
- State: Published
- Organisations: Stockholm University, University of Eastern Finland, University of Minho
- Contributors: Mayer, P., Schmidt, S. N., Annika, A., Mclachlan, M., Maenpaa, K., Lappanen, M.
Unified model for sorption, sequestration and degradation in soils and sediments

General information
State: Published
Organisations: Technical University of Denmark, Clarkson University, Aarhus University
Contributors: Trapp, S., Mayer, P., Rein, A.
Number of pages: 2
Publication date: 15 May 2011
Peer-reviewed: No
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http://milano.setac.eu/embed/Milan/AM11_extended_abstracts_1.pdf
Source: PXA Import
Source-ID: 37367631
Research output: Research › Paper – Annual report year: 2011

A Contaminant Trap as a Tool for Isolating and Measuring the Desorption Resistant Fraction of Soil Pollutants

Bioremediation of contaminated soils often leaves a desorption-resistant pollutant fraction behind in the soil, which in the present study was isolated with a combination of diffusive carrier and infinite diffusive sink. Such a diffusive sink was made by casting a composite of silicone and activated carbon into the bottom of a large glass. Field-contaminated soil samples were then suspended in a cyclodextrin solution and incubated in such glasses for the continuous trapping of PAH molecules during their release from the soil matrix. The PAH concentrations remaining in the soil were determined by exhaustive extraction and compared with a biodegradation experiment. The concentration decline in the first soil was faster in the contaminant trap than in the biodegradation experiment, but the halting of the biodegradation process before reaching the legal threshold level was well indicated by the contaminant trap. The PAH concentrations in the second soil hardly decreased in the traps at all, in good agreement with the biodegradation experiment. The PAHs in this soil appeared to be “stuck” by strong sorption. The contaminant trap proved to be a practical approach to the isolation and quantification of the desorption-resistant PAH fraction.

General information
State: Published
Organisations: Aarhus University, University of Natural Resources and Life Sciences, Vienna (BOKU)
Contributors: Mayer, P., Olsen, J. L., Gouliarmou, V., Hasinger, M., Kendler, R., Loibner, A. P.
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Impact factor 5.33
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BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
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ISI indexed (2012): ISI indexed yes
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Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945
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ISI indexed (2011): ISI indexed yes
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BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.86 SNIP 1.809
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
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Scopus rating (2007): SJR 2.774 SNIP 1.914
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.55 SNIP 1.893
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.608 SNIP 1.999
Web of Science (2005): Indexed yes
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Scopus rating (2003): SJR 2.54 SNIP 2.065
Web of Science (2003): Indexed yes
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Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.387 SNIP 1.968
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Application of passive dosing to study the biotransformation and biodegradation of hydrophobic compounds

Achieving well-defined and constant dissolved concentrations of hydrophobic compounds is challenging due to volatilization or sorptive losses. With passive dosing, continual partitioning into the test medium of compound(s) loaded in a polymer compensates for losses, and provides defined and constant dissolved concentrations. Passive dosing can be used for studying biotransformation/degradation. Here, the polymer HOC reservoir also compensates for losses due to the bio-transformation/degradation process itself. Furthermore, a large mass of test compound is introduced so that compound turnover is significant even at low dissolved concentrations thus facilitating measurement of the relevant endpoint (e.g., metabolic products in biotransformation or growth in biodegradation). This study details two applications of passive dosing for studying bio-transformation/degradation. A format has been developed to study the biodegradation of phenanthrene and fluoranthene by the bacterial strain EPA 505, allowing degradation rates to be quantified at defined freely dissolved concentrations from mg/L down to ng/L levels. Passive dosing was also applied for quantifying the mutagenicity of benzo(a)pyrene metabolites produced after activation by the liver S9 mix in the in vitro Ames II assay. Compared to the case with spiking, responses from passive dosing were shifted by a factor 100-1000 to lower concentrations, and were also more reproducible between repeated tests. This difference in apparent sensitivity cannot solely be explained by partitioning, and is due to slow dissolution kinetics as well as mass depletion of the spiked benzo(a)pyrene. Therefore, passive dosing is a useful tool for the study of hydrophobic compound biotransformation/degradation at well-defined dissolved concentrations down to very low levels. Important advantages include studying process kinetics at precisely defined dissolved concentrations and allowing increased compound turnover even at constant and low concentrations.

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Aquatic toxicity of PAHs and PAH mixtures at saturation to benthic amphipods: Linking toxic effects to chemical activity

Organisms in marine sediments are usually exposed to mixtures of polycyclic aromatic hydrocarbons (PAHs), whereas risk assessment and management typically focus on the effects of single PAHs. This can lead to an underestimation of risk if the effects of single compounds are additive or synergistic. Because of the virtually infinite number of mixture-combinations, and the many different targeted organisms, it would be advantageous to have a model for the assessment of mixture effects. In this study we tested whether chemical activity, which drives the partitioning of PAHs into organisms, can be used to model the baseline toxicity of mixtures. Experiments were performed with two benthic amphipod species (Orchomonella pinguis and Corophium volutator), using passive dosing to control the external exposure of single PAHs and mixtures of three and four PAHs. The baseline toxicity of individual PAHs at water saturation generally increased with increasing chemical activity of the PAHs. For O. pinguis, the baseline toxicity of PAH mixtures was successfully described by the sum of chemical activities. Some compounds and mixtures showed a delayed expression of toxicity, highlighting the need to adjust the length of the experiment depending on the organism. On the other hand, some of the single compounds had a higher toxicity than expected, possibly due to the toxicity of PAH metabolites. We suggest that chemical activity of mixtures can, and should, be used in addition to toxicity data for single compounds in environmental risk assessment. (C) 2011 Elsevier B.V. All rights reserved.

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Contributors: Engraff, M., Solere, C., Smith, K. E. C., Mayer, P., Dahllöf, I.
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Scopus rating (2016): CiteScore 4.38 SJR 1.627 SNIP 1.382
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Web of Science (2015): Indexed yes
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Scopus rating (2014): CiteScore 3.75 SJR 1.594 SNIP 1.324
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Scopus rating (2013): CiteScore 4.06 SJR 1.891 SNIP 1.485
Web of Science (2013): Impact factor 3.513
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.83 SJR 1.89 SNIP 1.489
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ISI indexed (2012): ISI indexed yes
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Web of Science (2011): Impact factor 3.761
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.798 SNIP 1.374
Web of Science (2010): Impact factor 3.333
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.014 SNIP 1.371
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.656 SNIP 1.337
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.651 SNIP 1.399
Scopus rating (2006): SJR 1.68 SNIP 1.405
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.448 SNIP 1.326
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.5 SNIP 1.372
Scopus rating (2003): SJR 1.547 SNIP 1.358
Web of Science (2003): Indexed yes
Crucial Role of Mechanisms and Modes of Toxic Action for Understanding Tissue Residue Toxicity and Internal Effect Concentrations of Organic Chemicals

This article reviews the mechanistic basis of the tissue residue approach for toxicity assessment (TRA). The tissue residue approach implies that whole-body or organ concentrations (residues) are a better dose metric for describing toxicity to aquatic organisms than is the aqueous concentration typically used in the external medium. Although the benefit of internal concentrations as dose metrics in ecotoxicology has long been recognized, the application of the tissue residue approach remains limited. The main factor responsible for this is the difficulty of measuring internal concentrations. We propose that environmental toxicology can advance if mechanistic considerations are implemented and toxicokinetics and toxicodynamics are explicitly addressed. The variability in ecotoxicological outcomes and species sensitivity is due in part to differences in toxicokinetics, which consist of several processes, including absorption, distribution, metabolism, and excretion (ADME), that influence internal concentrations. Using internal concentrations or tissue residues as the dose metric substantially reduces the variability in toxicity metrics among species and individuals exposed under varying conditions. Total internal concentrations are useful as dose metrics only if they represent a surrogate of the biologically effective dose, the concentration or dose at the target site. If there is no direct proportionality, we advise the implementation of comprehensive toxicokinetic models that include deriving the target dose. Depending on the mechanism of toxicity, the concentration at the target site may or may not be a sufficient descriptor of toxicity. The steady-state concentration of a baseline toxicant associated with the biological membrane is a good descriptor of the toxicodynamics of baseline toxicity. When assessing specific-acting and reactive mechanisms, additional parameters (e.g., reaction rate with the target site and regeneration of the target site) are needed for characterization. For specifically acting compounds, intrinsic potency depends on 1) affinity for, and 2) type of interaction with, a receptor or a target enzyme. These 2 parameters determine the selectivity for the toxic mechanism and the sensitivity, respectively. Implementation of mechanistic information in toxicokinetic-toxicodynamic (TK-TD) models may help explain time-delayed effects, toxicity after pulsed or fluctuating exposure, carryover toxicity after sequential pulses, and mixture toxicity. We believe that this mechanistic understanding of tissue residue toxicity will lead to improved environmental risk assessment. Integr Environ Assess Manag 2011;7:28-49. (C) 2010 SETAC
Equilibrium sampling of environmental pollutants in fish: Comparison with lipid-normalized concentrations and homogenization effects on chemical activity

Equilibrium sampling of organic pollutants into the silicone polydimethylsiloxane (PDMS) has recently been applied in biological tissues including fish. Pollutant concentrations in PDMS can then be multiplied with lipid/PDMS distribution coefficients (D-Lipid.PDMS) to obtain concentrations in fish lipids. In the present study, PDMS thin films were used for equilibrium sampling of polychlorinated biphenyls (PCBs) in intact tissue of two eels and one salmon. A classical exhaustive extraction technique to determine lipid-normalized PCB concentrations, which assigns the body burden of the chemical to the lipid fraction of the fish, was additionally applied. Lipid-based PCB concentrations obtained by equilibrium sampling were 85 to 106% (Norwegian Atlantic salmon), 108 to 128% (Baltic Sea eel), and 51 to 83% (Finnish lake eel) of those determined using total extraction. This supports the validity of the equilibrium sampling technique, while at the same time confirming that the fugacity capacity of these lipid-rich tissues for PCBs was dominated by the lipid fraction.

Equilibrium sampling was also applied to homogenates of the same fish tissues. The PCB concentrations in the PDMS were 1.2 to 2.0 times higher in the homogenates (statistically significant in 18 of 21 cases, p < 0.05), indicating that homogenization increased the chemical activity of the PCBs and decreased the fugacity capacity of the tissue. This observation has implications for equilibrium sampling and partition coefficients determined using tissue homogenates.

Environ. Toxicol. Chem. 2011;30:1515-1521. (C) 2011 SETAC

General information
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**Journal:** Environmental Toxicology and Chemistry

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Equilibrium Sampling of Persistent and Bioaccumulative Compounds in Soil and Sediment: Comparison of Two Approaches To Determine Equilibrium Partitioning Concentrations in Lipids

The equilibrium sampling in silicone is increasingly applied to measure freely dissolved concentrations and chemical activities within bioaccumulation research of hydrophobic organic chemicals. Two equilibrium methods were applied to PCB-contaminated soil and sediment, and directly calibrated with respect to equilibrium partitioning concentrations in lipids (C(lipid,partitioning)): (i) Solid phase microextraction in the headspace above the sample (HS-SPME) required optimization for its application to PCBs, and it was calibrated above external partitioning standards in olive oil. (ii) Equilibrium sampling with internally coated glass jars with varying thicknesses of silicone (PDMS) resulted in proportionality between coating and analyte mass, which confirmed several validity criteria. C(lipid,partitioning) was here determined as product of PDMS concentration and PDMS to lipid partition ratio. The results of the two methods were in good agreement and thus validated each other. Finally, the coated glass jar method was applied to field sediment containing invertebrates, which lead to C(lipid,partitioning) that were about two times higher than measured lipid-normalized concentrations in the organisms. Temperature differences and animal lipid structure were discussed as possible reasons for this discrepancy. Both methods combine high analytical performance, reduced equilibration times and new calibration possibilities, which makes them suited for bioaccumulation research and environmental monitoring.

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
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Web of Science (2016): Impact factor 6.198
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Occurrence of organochlorine pesticides in indoor dust
Organochlorine pesticides are present in the environment and suspected of causing serious health effects. Diet has been the main exposure source, but indoor source release is gaining focus. Within a monitoring study of polychlorinated biphenyls of Danish buildings built during the 1960s and 1970s, we coincidently determined extreme levels of dichlorodiphenyltrichloroethane (DDT) levels in two of ten random samples. This raises concern and further large scale investigations are warranted to confirm this.

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Contributors: Bräuner, E. V., Mayer, P., Gunnarsen, L., Vorkamp, K., Raaschou-Nielsen, O.
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.79 SJR 1.036 SNIP 0.967
Web of Science (2016): Impact factor 2.592
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.5 SJR 0.998 SNIP 0.923
Web of Science (2015): Impact factor 2.401
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.21 SJR 1.051 SNIP 1.047
Web of Science (2014): Impact factor 2.179
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.996 SNIP 0.949
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.023 SNIP 0.87
Web of Science (2012): Impact factor 2.085
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.954 SNIP 0.898
Web of Science (2011): Impact factor 1.991
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.994 SNIP 0.712
Web of Science (2010): Impact factor 1.81
BFI (2009): BFI-level 1
Sorption of phenanthrene in agricultural soils

Polycyclic aromatic hydrocarbons (PAH) are among the major contaminants in the terrestrial environment. The background level in normal agricultural land has increased for many years and it is expected to further increase in the future. Because of the very low water solubility and high Kow values, PAHs tend to sorb to the organic carbon (OC) in the soil.

This study aims to understand the contribution to phenanthrene sorption of various soils fractions such as organic carbon, clay, silt, and sand.

In 24 hours equilibrium sorption experiments, we determined the phenanthrene partition coefficient, KD for more than one hundred Danish and European agricultural top and sub soils (122 topsoils and 28 subsoils) as well as the normalized distribution coefficient of the organic carbon content (KOC), through single point isotherm measurements.

Possible effect of clay-complexed organic carbon was analyzed, as derived from the Dexter et al. (2008) n-index (ratio of clay to organic carbon of 10 kg kg^{-1}), on KOC, but we did not find it to markedly influence KOC nor be useful to better predict KOC for cultivated soils. Globally, the soils split into two groups with one group above and the other below the saturation line as defined by Dexter.

Top soils and subsoils showed different sorption behavior, with typically higher Koc for topsoils, likely due to different organic matter quality related to soil management and hydrological impact. Topsoils generally exhibited Koc values between the traditionally applied models of Abdul et al. and Karickhoff et al. These two models were documented useful to predict maximum and minimum Koc for agricultural topsoils, for example in regard to predicting long-term PAH leaching from cultivated areas. Furthermore, we suggest a new Koc model in between Abdul and Karickhoff for predicting average Koc for agricultural topsoils. Subsoils mostly followed Abdul, in agreement with that this model was developed for deeper soils and groundwater sediments lower in organic carbon (0.4 - 2%).

This study only concerns solid-liquid partitioning and thus the probability for PAH adsorption onto assumingly non-mobile soil particles. In perspective, the combined risk of dissolved PAH leaching and colloid-facilitated PAH leaching from cultivated land areas should be considered.

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Bioavailability of organochlorine compounds in aqueous suspensions of fullerene: Evaluated with medaka (Oryzias latipes) and negligible depletion solid-phase microextraction

The wide application of engineered nanomaterials, such as fullerene (C(60)), will inevitably lead to their release into the aqueous environment, which may alter the bioavailability of organic compounds to aquatic organisms. Negligible depletion solid-phase microextraction (nd-SPME) together with medaka (Oryzias latipes) bioaccumulation were used to study the effects of aqueous suspensions of fullerene (nC60) on the bioavailability of eight organochlorine compounds (OCCs) (log K(OW) 3.76-6.96). Freely dissolved concentrations of OCCs decreased by 11.5-88.4% at addition of 5 mg L(-1) nC60 as indicated by reduced equilibrium concentrations in the SPME fiber coating, the highest reduction being observed for the most hydrophobic OCCs. Medaka bioaccumulation study demonstrated that at the kinetic uptake regime, nC60 significantly decreased the bioaccumulation of the high hydrophobic OCCs (log K(OW) > 6), but slightly enhanced the bioaccumulation of the less hydrophobic OCCs (log K(OW) < 6). The OCC concentrations in medaka (C(fish)) at the kinetic uptake regime linearly correlated with that in nd-SPME fiber (C(fiber)) without nC60 (p = 0.007-0.013, R(2) = 0.666-0.723), but this correlation deteriorated with the presence of nC60 (p = 0.073-0.081, R(2) = 0.423-0.440). These results suggest that in nC60 the uptake mechanism of OCCs to medaka is different from that to nd-SPME fiber. While only the freely dissolved OCCs are available to nd-SPME fiber, both the freely dissolved and the nC60 associated OCCs contributed to the accumulation of OCCs to medaka. (C) 2010 Elsevier Ltd. All rights reserved.
Web of Science (2012): Indexed yes
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Web of Science (2011): Impact factor 3.206
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.879 SNIP 1.424
Web of Science (2010): Impact factor 3.155
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 1.842 SNIP 1.572
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.658 SNIP 1.58
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.5 SNIP 1.605
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.418 SNIP 1.673
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.479 SNIP 1.558
Web of Science (2005): Indexed yes
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.321 SNIP 1.323
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.902 SNIP 1.06
Web of Science (2002): Indexed yes
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Web of Science (2000): Indexed yes
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**Controlling and maintaining exposure of hydrophobic organic compounds in aquatic toxicity tests by passive dosing**

The risk assessment of hydrophobic organic compounds (HOCs) in aquatic toxicity or bioconcentration tests is a challenge due to their low aqueous solubilities, sorption and losses leading to poorly defined exposure and reduced test sensitivity. Passive dosing overcomes these problems via the continual partitioning of HOCs from a dominating reservoir loaded in a biocompatible polymer such as silicone, providing defined and constant freely dissolved concentrations and eliminating spiking with co-solvents. This study characterised the performance of a passive dosing format for aquatic tests with small organisms such as invertebrates and algae, consisting of PDMS silicone cast into the base of the glass test vessel. The PDMS silicone was loaded by partitioning from a methanol solution containing PAHs (log K(OW) 3.56-6.63) as model compounds, followed by removal of the methanol with water. This resulted in highly reproducible PDMS silicone HOC concentrations. When shaking, release of PAHs into aqueous solution was rapid and reproducible, and equilibrium partitioning was reached within 5 h for all compounds. The buffering capacity was sufficient to maintain stable concentrations over more than 10 weeks. This format was applied in a 48 h Daphnia magna immobilisation assay to test the toxicity of a range of PAHs at their aqueous solubility. D. magna immobilisation did not show a trend with aqueous solubility or hydophobicity (K(OW)) of the PAHs. However, the immobilisation data for all compounds could be fitted with one maximum chemical activity response curve. Those PAHs with the lowest maximum chemical activities resulted in no immobilisation. Naphthalene and phenanthrene showed full toxicity at aqueous solubility, and passive dosing was also used for the concentration-response testing of these compounds. The freely dissolved aqueous concentrations causing 50% immobilisation (EC-50) were 1.96 mg L(-1) for naphthalene and 0.48 mg L(-1) for phenanthrene. Therefore, passive dosing is a practical and economical means of improving the exposure of HOCs in aquatic toxicity or bioconcentration tests.
Do complex matrices modify the sorptive properties of polydimethylsiloxane (PDMS) for non-polar organic chemicals?

The partitioning of non-polar analytes into the silicone polydimethylsiloxane (PDMS) is the basis for many analytical approaches such as solid phase microextraction (SPME), stir bar sorptive extraction (SBSE) and environmental passive sampling. Recently, the methods have been applied to increasingly complex sample matrices. The present work investigated the possible effect of complex matrices on the sorptive properties of PDMS. First, SPME fibers with a 30 μm PDMS coating were immersed in 15 different matrices, including sediment, suspensions of soil and humic substances, mayonnaise, meat, fish, olive oil and fish oil. Second, the surface of the fibers was wiped clean, and together with matrix-free control fibers, they were exposed via headspace to 7 non-polar halogenated organic chemicals in spiked olive oil. The fibers were then solvent-extracted, analyzed, and the ratios of the mean concentrations in the matrix-immersed fibers to the control fibers were determined for all matrices. These ratios ranged from 92% to 112% for the four analytes with the highest analytical precision (i.e. polychlorinated biphenyls (PCBs) 3, 28, 52 and brominated diphenyl ether (BDE) 3), and they ranged from 74% to 133% for the other three compounds (i.e. PCBs 101, 105 and gamma-hexachlorocyclohexane (HCH)). We conclude that, for non-polar, hydrophobic chemicals, the sorptive properties of the PDMS were not modified by the diverse investigated media and consequently that PDMS is suited for sampling of these analytes even in highly complex matrices. (C) 2010 Elsevier B.V. All rights reserved.
Low accessibility and chemical activity of PAHs restrict bioremediation and risk of exposure in a manufactured gas plant soil
Composting of manufactured gas plant soil by a commercial enterprise had removed most of its polycyclic aromatic hydrocarbons (PAHs), but concentrations remained above regulatory threshold levels. Several amendments and treatments were first tested to restart the PAH degradation, albeit with little success. The working hypothesis was then that PAHs were “stuck” due to strong sorption to black carbon. Accessibility was measured with cyclodextrin extractions and on average only 4% of the PAHs were accessible. Chemical activity of the PAHs was measured by equilibrium sampling, which confirmed a low exposure level. These results are consistent with strong sorption to black carbon (BC), which constituted 59% of the total organic carbon. Composting failed to remove the PAHs, but it succeeded to minimize PAH accessibility and chemical activity. This adds to accumulating evidence that current regulatory thresholds based on bulk concentrations are questionable and alternative approaches probing actual risk should be considered. (C) 2010 Elsevier Ltd. All rights reserved.
Original language: English
Keywords: Soot, Biodegradation, Hydrophobic organic pollutants, Freely dissolved concentrations, Persistence

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More of EPA's SPARC Online Calculator: The Need for High-Quality Predictions of Chemical Properties

General information
State: Published
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Passive Dosing for Producing Defined and Constant Exposure of Hydrophobic Organic Compounds during In Vitro Toxicity Tests

Toxicity testing of hydrophobic organic compounds (HOCs) in plastic cell culture plates is problematic due to compound losses through volatilization and sorption to the wells and culture medium constituents. This leads to poorly defined exposure and reduced test sensitivity. Passive dosing can overcome these problems by the continual partitioning of HOCs from a dominating reservoir loaded in a biologically inert polymer such as silicone, providing defined and constant freely dissolved concentrations and also eliminating spiking with cosolvents. This study aimed to select a suitable passive dosing format for in vitro tests in multiwell plates and characterize its performance at 37 degrees C. Silicone O-rings were the most suitable format, as they were both practical and demonstrated excellent passive dosing performance. (1) The rings were loaded by partitioning from a methanol solution containing polycyclic aromatic hydrocarbons (PAHs) (log K(OW), 3.33-6.43) that served as model compounds, followed by removal of the methanol with water. This resulted in highly reproducible HOC concentrations in the silicone O-rings. (2) The release of PAHs into aqueous solutions was rapid and reproducible, with equilibrium partitioning being reached within hours. (3) The buffering capacity of the O-rings was sufficient to maintain stable concentrations over more than 72 h. The O-rings were then applied to test a range of PAHs at their aqueous solubility in all arrays of established in vitro cell culture assays with human cells and cell lines. These included the formation of reactive oxygen species, induction of the IL-8 cytokine promoter, and secretion of MCF-1 by the cells. The biological responses depended on the melting point of the individual PAHs and their maximum chemical activities (a(max)). Only those PAHs with the highest a(max) stimulated the formation of reactive oxygen species and MCP-1 secretion, while they inhibited the induction of the IL-8 cytokine promoter.

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Contributors: Smith, K. E., Oostingh, G. J., Mayer, P.
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Web of Science (2017): Impact factor 3.432
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.36 SJR 1.187 SNIP 1.057
Web of Science (2016): Impact factor 3.278
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.7 SJR 1.301 SNIP 1.147
Web of Science (2015): Indexed yes
Passive Dosing to Determine the Speciation of Hydrophobic Organic Chemicals in Aqueous Samples
A new analytical approach to determine the speciation of hydrophobic organic analytes is presented. The freely dissolved concentration in a sample is controlled by passive dosing from silicone (poly(dimethylsiloxane)), and the total sample concentration at equilibrium is measured. The free fraction is determined as the ratio between measured concentrations in pure water and sample. C-14-labeled fluoranthene served as model analyte, and total sample concentrations were easily measured by liquid scintillation counting. The method was applied to surface water, stormwater runoff, and wastewater. In the untreated wastewater, 61% of the fluoranthene was bound to suspended solids, 28% was associated to dissolved organic matter, and 11% was freely dissolved, while in treated wastewater, the speciation was 16% bound to suspended solids, 4% bound to dissolved organic matter, and 80% freely dissolved. The free fraction in roof runoff (85%) and surface water (91%) was markedly higher than in runoff from paved areas, which ranged from 27 to 36%. A log K-DOC value of 5.26 was determined for Aldrich humic acid, which agrees well with reported values obtained by fluorescence quenching and solid phase microextraction (SPME). This analytical approach combines simplicity with high precision, and it does not require any phase separation steps.
Response to Comment on "More of EPA's SPARC Online Calculator - The Need for High Quality Predictions of Chemical Properties"

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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Web of Science (2015): Impact factor 5.393
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Impact factor 5.33
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BFI (2013): BFI-level 2
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Web of Science (2013): Impact factor 5.481
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Web of Science (2013): Indexed yes
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Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Web of Science (2012): Impact factor 5.257
Combined chemical (fluoranthene) and drought effects on lumbricus rubellus demonstrate the applicability of the independent action model for multiple stressor assessment

The combined effect of a chemical (fluoranthene) and a nonchemical stress (reduced soil moisture content) to the widely distributed earthworm Lumbricus rubellus were investigated in a laboratory study. Neither fluoranthene (up to 500 μg/g) nor low soil moisture (15% below optimal) had a significant effect on the survival of the exposed worms, but a significant effect on reproduction (cocoon production rate) was found for both stressors (p < 0.001 in both cases). The response of cocoon production to each stressor could be well described by a logistic model; this suggested that the joint effects may be applicable to description using the independent action (IA) model that is widely used in pharmacology and chemical mixture risk assessment [1]. Fitting of the IA model provided a good description of the combined stressor data (accounting for 53.7% of total variation) and was the most parsimonious model describing joint effect (i.e., the description of the data was not improved by addition of further parameters accounting for synergism or antagonism). Thus, the independent action of the two responses was further supported by measurement of internal fluoranthene exposure. The chemical activity of fluoranthene in worm tissue was correlated only with soil fluoranthene concentration and not with soil moisture content. Taken together these results suggest that the IA model can help interpret the joint effects of chemical and nonchemical stressors. Such analyses should, however, be done with caution since the literature data set suggests that there may be cases where interactions between stressors result in joint effects that differ significantly from IA predictions.
Development of a dynamic delivery method for in vitro bioassays

Measuring the biological activity of hydrophobic chemicals using in vitro assays is challenging because their aqueous solubility is low and the high density of bio-suspensions strongly decreases the bioavailability of hydrophobic pollutants. Dynamic dosing by partitioning from a stable polymer has a potential to overcome these limitations. Poly(dimethylsiloxane) (PDMS) was chosen due to its documented bio-compatibility and excellent partitioning properties. PDMS sheets were loaded with five polycyclic aromatic hydrocarbons (PAHs) and then immersed in model bio-suspensions composed of membrane vesicles ("chromatophores", composed of 30% lipids and 70% proteins) isolated from the photosynthetic bacterium Rhodobacter sphaeroides or phospholipid bilayer vesicles (liposomes) composed of palmitoyloleoyl phosphatidylcholine (POPC). Method development included the determination of partition coefficients between chromatophores or liposomes and water, desorption rate constants from PDMS to bio-suspensions, and diffusion resistances in both PDMS and bio-suspensions. The release of the PAHs from the PDMS into the bio-suspensions was measured and modeled as a combination of diffusion in pure water and diffusion in a completely mixed solvent composed of water and bio-suspensions. The mass transfer resistance for the release was lower in the PDMS than in the tested solutions, which demonstrates that PDMS can efficiently deliver PAHs even to dense biosuspensions. The contribution of aqueous diffusion to the mass transfer decreased with increasing hydrophobicity of the PAHs indicating that hydrophobic chemicals are efficiently transported with suspended biomaterial. The passive dosing system is versatile and offers a number of applications. Promising are tests with instantaneous response, where the time-dependent effect can be translated to concentration-effect curves but the system is also applicable for assuring constant dosing for longer-term testing. (C) 2009 Elsevier Ltd. All rights reserved.
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Effect of vegetable oil addition on bioaccessibility and biodegradation of polycyclic aromatic hydrocarbons in historically contaminated soils

BACKGROUND: Bioaccessibility is often the limiting factor for the biodegradation of polycyclic aromatic hydrocarbons (PAH) in soils. The present study explores the potential of amending canola oil, an economically and ecologically attractive soil additive, for the enhancement of bioaccessibility and, in consequence, biodegradation of PAH in historically contaminated, bioaccessibility limited soils.

RESULTS: The amendment of canola oil (1% and 5%, w/w) to contaminated soils increased the bioaccessibility and the subsequent biodegradation of PAH with up to four rings. Residual concentrations of pyrene and fluoranthene in oil-treated soils were 38-53% lower compared to the unamended tests. The continuous removal of bioaccessible PAH with a passive sampling system confirmed that oil amendment indeed increased bioaccessibility, leading to a lower non-accessible PAH fraction. Canola oil amendment did, by contrast, not increase the bioaccessibility of high molecular weight PAH, likely due to their strong binding to soil organic carbon compounds.

CONCLUSION: Canola oil can be used efficiently in low concentrations to render PAH up to four rings accessible for biodegradation in historically contaminated soils. Contaminants remaining in soil after treatment may pose a significantly lowered environmental risk, as is indicated by the lack of mobilisation by a solubilising agent such as canola oil. (C) 2009 Society of Chemical Industry
Equilibrium sampling through membranes (ESTM) of acidic organic pollutants using hollow fibre modules in continuous steady-state mode

Hollow fibre (HF) membrane modules were applied in continuous mode for equilibrium sampling through membranes (ESTIM) of polar organic pollutants. Phenolic compounds (chlorophenols, cresols and phenol) served as model substances and ESTM was tuned towards the measurement of freely dissolved concentrations (C\(\text{free}\)). HF membrane modules were constructed using thin-walled membrane, 1-m module length and low packing density in order to optimise the uptake kinetics of the analytes into the acceptor solution. Such custom made devices were tested and compared to commercially available modules. The former modules performed best for continuous ESTIM. The custom made modules provided steady-state equilibrium within 20-40 min and enrichment that was in general agreement with calculated distribution ratios between acceptor and sample. In experiments during which sample concentration was changed, acceptor response time to decreased sample concentration was around 30 min for custom built modules. In the presence of commercial humic acids, analytes showed lower steady-state enrichment, which is due to a decrease in C\(\text{free}\). Continuous ESTM may be automated and is suggested for use in online determination of C\(\text{free}\) of pollutants and studies...
on sorption of pollutants. Future studies should include optimisation of the membrane liquid and factors regarding the residence time of the acceptor solution in the fibre lumen. Qualitative aspects of DOM should also be included, as natural DOM can be fractionated. C\(_{\text{free}}\) could be correlated to DOM properties that have previously been shown to influence sorption, such as aromaticity, carboxylic acid content and molecular size. (C) 2009 Elsevier Ltd. All rights reserved.
Scopus rating (2009): SJR 1.842 SNIP 1.572
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.658 SNIP 1.58
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.5 SNIP 1.605
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.418 SNIP 1.673
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.479 SNIP 1.558
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.627 SNIP 1.479
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.321 SNIP 1.323
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.902 SNIP 1.06
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Scopus rating (2001): SJR 0.924 SNIP 0.978
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.959 SNIP 0.871
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.022 SNIP 0.844
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In Situ Silicone Tube Microextraction: A New Method for Undisturbed Sampling of Root-exuded Thiophenes from Marigold (Tagetes erecta L.) in Soil

The difficulties of monitoring allelochemical concentrations in soil and their dynamics over time have been a major barrier to testing hypotheses of allelopathic effects. Here, we evaluate three diffusive sampling strategies that employ polydimethylsiloxane (PDMS) sorbents to map the spatial distribution and temporal dynamics of root-exuded thiophenes from the African marigold, Tagetes erecta. Solid phase root zone extraction (SPRE) probes constructed by inserting stainless steel wire into PDMS tubing were used to monitor thiophene concentrations at various depths beneath marigolds growing in PVC pipes. PDMS sheets were used to map the distribution of thiophenes beneath marigolds grown in thin glass boxes. Concentrations of the two major marigold thiophenes measured by these two methods were extremely variable in both space and time. Dissection and analysis of roots indicated that distribution of thiophenes in marigold roots also was quite variable. A third approach used 1 m lengths of PDMS microtubing placed in marigold soil for repeated sampling of soil without disturbance of the roots. The two ends of the tubing remained out of the soil so that solvent could be washed through the tubing to collect samples for HPLC analysis. Unlike the other two methods, initial experiments with this approach show more uniformity of response, and suggest that soil concentrations of marigold thiophenes are affected greatly even by minimal disturbance of the soil. Silicone tube microextraction gave a linear response for alpha-terthienyl when maintained in soils spiked with 0-10 ppm of this thiophene. This method, which is experimentally simple and uses inexpensive materials, should be broadly applicable to the measurement of non-polar root exudates, and thus provides a means to test hypotheses about the role of root exudates in plant-plant and other interactions.

General information
State: Published
Organisations: Ashland University, University of Copenhagen
Contributors: Mohney, B. K., Matz, T., LaMoreaux, J., Wilcox, D. S., Gimsing, A. L., Mayer, P., Weidenhamer, J. D.
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Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Ecology
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Matrix solid-phase microextraction for measuring freely dissolved concentrations and chemical activities of PAHs in sediment cores from the western Baltic Sea

Sediment-pore water partitioning of polycyclic aromatic hydrocarbons (PAHs) was studied in sediment cores of a dumping area in the western Baltic Sea and compared to a reference site. Freely dissolved concentrations \( C_{\text{free}} \) of nine PAHs were measured in sediment samples using solid-phase microextraction (SPME), a cost and time-efficient method with detection limits in the lower ng L\(^{-1} \) range. Elevated levels of \( C_{\text{free}} \) were measured at the dumping site, where concentration peaks in the core correlated with the presence of the dumped material, which was conspicuous in its color and consistency. Sediment concentrations of PAHs were three orders of magnitude higher at the dumping site than at the reference site, whereas \( C_{\text{free}} \) was only one order of magnitude greater. Chemical activities of the PAHs in the sediment cores were calculated from \( C_{\text{free}} \) to predict the baseline toxic potential of the contaminant mixture. Finally, gradients in \( C_{\text{free}} \) and chemical activity were used to determine the direction of diffusion within the sediment and to obtain a spatial characterization of the PAH exposure. \( C_{\text{free}} \) and chemical activity are important exposure parameters for the prediction of bioconcentration and toxicity in sediment organisms, and their measurement should be included in risk-assessment and pollution-management strategies. (C) 2008 Elsevier Ltd. All rights reserved.

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Organisations: Leibniz Institute for Baltic Sea Research Warnemünde (IOW), Aarhus University
Contributors: Witt, G., Liehr, G. A., Borck, D., Mayer, P.
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.39 SJR 1.447 SNIP 1.625
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BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.04 SJR 1.497 SNIP 1.567
Web of Science (2015): Impact factor 3.698
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Scopus rating (2013): CiteScore 3.92 SJR 1.721 SNIP 1.751
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BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.5 SJR 1.794 SNIP 1.618
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Web of Science (2012): Indexed yes
Measuring Pyrethroids in Sediment Pore Water using Matrix-solid Phase Microextraction

Pyrethroids are hydrophobic insecticides commonly used in both agricultural and urban environments. Their high toxicity to aquatic organisms, including benthic invertebrates, and detection in the sediment at many locations in California, USA, have spawned interest in understanding their bioavailability in bed sediments. A recent study showed good correlation between uptake of C-14-permethrin in Chironomus tentans and solid-phase microextraction (SPME) fibers in sediments. The present study was directed at the development of an SPME technique applicable to trace levels of nonlabeled pyrethroids in sediment. Disposable polydimethylsiloxane fibers were used to detect freely dissolved pore-water concentrations of bifenthrin, fenpropathrin, cis-permethrin, trans-permethrin, cyfluthrin, cypermethrin, and esfenvalerate under agitated and static conditions. Partition equilibrium between fiber and sediment was reached in <5 d when the samples were agitated on a shaker at low speed, while much longer times (>23 d) were needed without agitation. Polydimethylsiloxane to water partition ratios (K-PDMS) of the seven pyrethroids were measured separately and ranged from 2.83 x 10(5) to 1.89 x 10(6). When applied to field-contaminated sediments, agitated matrix-SPME was able to detect pore-water concentrations as low as 0.1 ng/L. The method developed in the present study may be coupled with bioassays to gain mechanistic understanding of factors affecting pyrethroid toxicities, and applied to field samples to better predict sediment toxicities from pyrethroid contamination.

General information
State: Published
Organisations: University of California, Aarhus University
Possibilities and limitations of equilibrium sampling using polydimethylsiloxane in fish tissue

Polydimethylsiloxane (PDMS) has been used for passive equilibrium sampling in numerous abiotic environmental matrices. Recently, this approach was extended to lipid-rich tissue. This work investigated the possibilities and limitations of using PDMS thin-film extraction for in tissue equilibrium sampling in fish species of varying lipid content. Polychlorinated biphenyls (PCBs) were used as model lipophilic organic pollutants. PDMS thin-films were inserted in intact fish tissue for differing time periods (1 h up to 1 week). The thin-films were then solvent-extracted and the extracts were analyzed using gas chromatography coupled to mass spectrometry. Whether equilibrium had been established was investigated either by using PDMS thin-films of multiple thicknesses (140-620 μm) or by assessing kinetics by means of time series. Equilibration was found to be rapid (i.e. in the range of hours) in lipid-rich fish whereas equilibrium was not achieved within one week in tissues with low or medium lipid content (i.e. up to 2% lipids). Regarding lipid-rich fish, the newly developed method was found to be sufficiently sensitive to determine equilibrium partitioning concentrations of PCBs in lipids of samples from the Baltic Sea, and it is a promising approach for any kind of fatty tissue. (C) 2009 Elsevier Ltd. All rights reserved.

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Organisations: Stockholm University, Aarhus University
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Ratings:
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BFI (2017): BFI-level 2
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Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.479 SNIP 1.558
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.627 SNIP 1.479
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.321 SNIP 1.323
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.902 SNIP 1.06
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.924 SNIP 0.978
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.959 SNIP 0.871
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.022 SNIP 0.844

Original language: English
Keywords: In tissue equilibrium sampling, Silicone thin-film extraction, Internal exposure, Solid Phase Microextraction (SPME), Persistent organic pollutants (POPs), Environmental monitoring
Silicone Membrane Equilibrator: Measuring Chemical Activity of Nonpolar Chemicals with Poly(dimethylsiloxane) Microtubes Immersed Directly in Tissue and Lipids

The chemical activity of organic chemicals directs their diffusion and partitioning and is consequently crucial for their transport, distribution, and toxic effects. A silicone membrane equilibrator is introduced for measuring the chemical activity of nonpolar organic chemicals in lipid rich samples: (I) A 6 m poly(dimethylsiloxane) (PDMS) microtube (300 μm i.d., 640 μm o.d.) was placed in a sample, and a sample-PDMS equilibrium was reached within 10 min for 12 polycyclic aromatic hydrocarbons (PAHs) acting as model compounds. (II) A plug of 100 μL of methanol was pushed through the tube to equilibrate it with the PDMS and thus the sample. (III) This yielded an undiluted methanol extract that was injected into a high-performance liquid chromatograph (HPLC) with multiband fluorescence detection. Quantification limits expressed as unitless chemical activities ranged from 6 x 10(-9) to 5 x 10(-8), and relative standard deviations were from 6% to 19%. Chemical activities of PAHs in mussels from two polluted sites were measured between 10(-7) and 10(-5), and activity coefficients for PAHs in vegetable and fish oils hardly differed between oils. This method can be used for internal exposure measurements, for monitoring product safety/conformity, and process control. The method can also be applied to measure total analyte concentrations in lipid-rich samples and oils.

General information
State: Published
Organisations: Aarhus University, Lund University
Contributors: Mayer, P., Toräng, L., Glæsner, N., Jönsson, J. Å.
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Publication information
Journal: Analytical Chemistry
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Issue number: 4
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.24
Web of Science (2017): Impact factor 6.042
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.08
Web of Science (2016): Impact factor 6.32
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6
Web of Science (2015): Impact factor 5.886
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.79
Web of Science (2014): Impact factor 5.636
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.01
Web of Science (2013): Impact factor 5.825
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.8
Web of Science (2012): Impact factor 5.695
ISI indexed (2012): ISI indexed yes
Determination of the chemical activity of hydrophobic organic compounds in soil using polymer coated vials

Background: In soils contaminated by hydrophobic organic compounds, the concentrations are less indicative of potential exposure and distribution than are the associated chemical activities, fugacities and freely dissolved concentrations. The latter can be measured by diffusive sampling into thin layers of polymer, as in, for example, solid phase micro-extraction. Such measurements require equilibrium partitioning of analytes into the polymer while ensuring that the sample is not depleted. We introduce the validation of these requirements based on parallel sampling into polymer layers of different thicknesses.

Results: Equilibrium sampling devices were made by coating glass vials internally with 3-12 μm thick layers of polydimethylsiloxane (PDMS). These were filled with slurries of a polluted soil and gently agitated for 5 days. The concentrations of 7 polycyclic aromatic hydrocarbons (PAHs) in the PDMS were measured. Validation confirmed fulfilment of the equilibrium sampling requirements and high measurement precision. Finally, chemical activities of the PAHs in the soil were determined from their concentrations and activity coefficients in the PDMS.

Conclusion: PAHs' thermodynamic activities in a soil test material were determined via a method of uptake into PDMS. This can be used to assess chemical exposure and predict diffusion and partitioning processes.
Device and Method for Isolation, Concentration and/or Identification of Compounds

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State: Published
Organisations: Aarhus University
Contributors: Mayer, P., Reichenberg, F., Toräng, L.
Publication date: 2008

Publication information
Country: Denmark
IPC: BO1L 3/14 (2006.01)
Date: 25/09/2008
Equilibrium sampling: Partitioning of organochlorine compounds from lipids into polydimethylsiloxane

Polydimethylsiloxane (PDMS) can be used for equilibrium sampling of environmental pollutants in a large variety of matrices including biota. For comparison with lipid-normalized concentrations e.g. from biota monitoring programmes, reliable lipid to PDMS partition ratios K(Lipid,PDMS) are required. Addition, ally, K(Lipid,PDMS) facilitate comparison of equilibrium sampling data obtained in various environmental media and can be helpful to convert equilibrium sampling data into a more informative form. This work investigated the equilibrium partitioning of polychlorinated biphenyls (PCBs) and selected organochlorine pesticides (OCPs) between lipids from biota of different trophic levels and PDMS. One vegetable oil, a fish oil and seal oil were investigated. The lipid to PDMS partition ratios were compound-specific and ranged from 14.5 to 62.9 g/g with correction for lipid uptake into the PDMS and from 13.0 to 54.8 g/g without correction. Additionally, PDMS served as a reference partitioning phase for the accurate determination of lipid to lipid partition ratios, which for all analytes were close to unity. Evaluating the results in a bioaccumulation context, they indicate that the equilibrium partitioning of neutral lipophilic environmental contaminants into the lipids of the three investigated species will be very similar, although they represent three distinct trophic levels. (C) 2008 Elsevier Ltd. All rights reserved.
Field Testing of Equilibrium Passive Samplers to Determine Freely Dissolved Native Polycyclic Aromatic Hydrocarbon Concentrations

Equilibrium passive samplers are promising tools to determine freely dissolved aqueous concentrations (C-W,C-free) of hydrophobic organic compounds. Their use in the field, however, remains a challenge. In the present study on native polycyclic aromatic hydrocarbons (PAHs) in Oslo Harbor, Norway, two different passive sampler materials, polyoxymethylene (POM; thickness, 55 μm [POM-55] and 500 μm [POM-500]) and polydimethylsiloxane (PDMS; thickness, 200 μm), were used to determine in the laboratory C-W,C-free in sediment pore water (C-PW,C-free), and the suitability of five passive samplers for determination of C-W,C-free in overlying surface water was tested under field conditions. For laboratory determinations of C-PW,C-free, both POM-55 and PDMS (thickness, 28 μm coatings on solid-phase microextraction fibers, with PDMS tubing as a good alternative. Low-density polyethylene (thickness, 100 μm) and POM-500 did not reach equilibrium within 119 d in the field. Realistic values were obtained for dissolved organic carbon-water partition coefficients in the field (approximately one log unit under log K-OW), which strengthened the conclusion that equilibrium was established in field-exposed passive samplers. At all four stations, chemical activity ratios between pore water and overlying water were greater than one for all PAHs, indicating that the sediment was a PAH diffusion source and that sediment remediation may be an appropriate treatment for PAH contamination in Oslo Harbor.
Immersed solid phase microextraction to measure chemical activity of lipophilic organic contaminants in fatty tissue samples

It is known that solid phase microextraction (SPME) fibers can be equilibrated directly within environmental matrices such as water, sediment and soil slurries. Here it is shown that this method can also be applied to biological tissue. SPME extraction of biological matrices reportedly causes lipophilic fouling of the fiber. However, we found no significant measurement bias when combining equilibrium sampling with fiber surface cleaning. The uptake of lipophilic organic pollutants from the tissue and into the SPME fiber coating was characterized by fast equilibrium partitioning without sample depletion and without impacting the sorptive properties of the fiber. The precision of the method when applied to hexachlorobenzene and several PCB congeners in harbor porpoise blubber was 15%, which includes the variation between SPME samplings, manual injections and the instrumental analysis. A good correlation ($r^2 = 0.95$) was obtained between SPME measurements of PCB 153 in blubber and concentrations obtained via a traditional analytical approach. These results indicate that SPME is a promising technique for measuring chemical activity in biological tissue, which would make it a useful tool for studying chemical distribution in organisms as well as biodilution and biomagnification phenomena. (C) 2007 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Leibniz Institute for Baltic Sea Research Warnemunde (IOW), Aarhus University
Contributors: Ossiander, L., Reichenberg, F., McLachlan, M. S., Mayer, P.
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Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Chemosphere
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.62 SJR 1.435 SNIP 1.448
Web of Science (2017): Impact factor 4.427
Web of Science (2017): Indexed yes
Impacts of some Environmentally Relevant Parameters on the Sorption of Polycyclic Aromatic Hydrocarbons to Aqueous Suspensions of Fullerene

The wide application of engineered carbon nanomaterials (CNMs), such as fullerene (C(60)), inevitably will result in their introduction into the aqueous environment. It is likely CNMs will associate with abundant natural organic matter (NOM) and engineered surfactants to form stable aqueous suspensions through various environmental processes. The present study reveals that sorption of polycyclic aromatic hydrocarbons (PAHs) to fullerene resulted in a remarkable decline of freely dissolved PAH concentrations. For the three PAHs studied (phenanthrene, fluoranthene, and chrysene) with log K(OW) in the range of 4.56 to 5.81, the measured sorption coefficients to aqueous suspensions of fullerene (log K(C60) = 4.71 - 5.48) were close to that of dissolved organic carbon (DOC) from Aldrich humic acid (log K(DOC) = 4.48 - 5.91).

Aqueous suspensions of fullerene were stable for a wide range of pH (3.0 - 11.0) and salinity conditions (0 - 25 mM NaCl), and the pH and salinity had minor effects on the sorption of PAHs to aqueous suspensions of fullerene. The addition of humic acids (5 mg/L DOC) to the fullerene (5 mg/L) suspensions resulted in an additional reduction of freely dissolved PAH concentrations. The high PAH sorption coefficients to suspended fullerene suggest that the release of fullerene to the aquatic environment might affect PAH fate and exposures.
Isomer-Specific Biodegradation of Methylphenanthrenes by Soil Bacteria

It is assumed that bacteria generally degrade 2-methylphenanthrene (2MPhe) in preference to 1-methylphenanthrene (1MPhe), and that environmental biodegradation of methylated PAHs therefore can be described qualitatively by changes in relative concentrations of these isomers. Our objective was to investigate whether microbial phenanthrene degraders (Sphingomonas and Mycobacterium) show such isomer-specific PAH degradation. Eleven out of twenty-nine phenanthrene degraders could grow on methylphenanthrene. The mycobacteria grew only on 2MPhe, the sphingomonads grew mostly on 1MPhe, and one sphingomonad could utilize both substrates. Seven strains were tested in a two-phase system where 1MPhe and 2MPhe were supplied in heptamethylnonane. For these strains, a consistent description of biodegradation based on the 2MPhe/1MPhe diagnostic ratio would not be possible because three Mycobacterium and one Sphingomonas degraded 2MPhe faster than 1MPhe, another Sphingomonas degraded 1MPhe and 2MPhe at almost equal rates, and two Sphingomonas degraded 1MPhe than 2MPhe. Thus, environmental biodegradation of phenantherenes may theoretically proceed with only minor changes in 2MPhe/1MPhe ratios if individual members of the degrader community have different isomer preferences. However, two soil microcosms polluted with bunker oil confirmed...
the general decline in 2MPhe/1MPhe ratio during oil biodegradation.

**General information**

State: Published  
Organisations: Geological Survey of Denmark and Greenland, Roskilde University, Aarhus University, University of Copenhagen  
Contributors: Lamberts, R. F., Christensen, J. H., Mayer, P., Andersen, O., Johnsen, A. R.  
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Peer-reviewed: Yes

**Publication information**

Journal: Environmental Science & Technology (Washington)  
Volume: 42  
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Ratings:  
BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941  
Web of Science (2017): Impact factor 6.653  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902  
Web of Science (2016): Impact factor 6.198  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838  
Web of Science (2015): Impact factor 5.393  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003  
Web of Science (2014): Impact factor 5.33  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102  
Web of Science (2013): Impact factor 5.481  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043  
Web of Science (2012): Impact factor 5.257  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945  
Web of Science (2011): Impact factor 5.228  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 2.979 SNIP 1.726  
Web of Science (2010): Impact factor 4.827  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 2.86 SNIP 1.809
Multivariate Analysis of Selected Metal Ion Transport through a Hollow-Fiber Supported Liquid Membrane Device used for Passive Sampling Monitoring

A hollow fiber supported liquid membrane module using one single fiber impregnated with a mixture of 1,10-dibenzy1-1,10-diaza-18-crown-6 and bis(2-ethylhexyl)phosphate dissolved in hexylbenzene was used for passive sampling of ppb levels of Pb(II), Cu(II), Zn(II), Mn(II), Ni(II), and Cd(II) in water. The target ions were simultaneously transported and preconcentrated into a citric acid acceptor solution within the lumen of the hollow fiber with enrichment factors between 5 and 4000 times. A multivariate analysis of several physical and chemical parameters that affect transport was performed. Under conditions of constant concentration profiles a more robust performance of the device was observed.

General information
State: Published
Organisations: National Autonomous University of Mexico, Chinese Academy of Sciences, Lund University, Danish Centre for Environment and Energy
Contributors: Rodríguez de San Miguel, E., Liu, J., Mayer, P., Jönsson, J. Å.
Pages: 602-623
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Solvent Extraction and Ion Exchange
Volume: 26
Issue number: 5
ISSN (Print): 0736-6299
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.22 SJR 0.85 SNIP 1.117
Web of Science (2017): Impact factor 2.034
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.36 SJR 0.672 SNIP 1.449
Passive Dosing of Soil Invertebrates with Polycyclic Aromatic Hydrocarbons: Limited Chemical Activity Explains Toxicity Cutoff

The partitioning of organic soil pollutants into soil organisms is driven by their chemical activity, which normally does not exceed that of the pure pollutant. Passive dosing with the silicone poly(dimethylsiloxane) (PDMS) was used to initiate and maintain the maximum chemical activity of 10 polycyclic aromatic hydrocarbons (PAHs) in toxicity tests with the springtail Folsomia candida. The test animals could move freely on the PDMS saturated with PAHs, resulting in direct contact and exposure to saturated air. After 7 days, springtail lethality correlated neither with the octanol-water partition coefficients of the PAHs nor with their molecular size, but with their melting point. All low-melting PAHs ($T(M) \leq 110$ degrees C) caused 100% lethality, whereas all high-melting PAHs ($T(M) \geq 180$ degrees C) caused no significant lethality. The lethality was successfully fitted to one chemical activity response curve for all PAHs tested, with effective chemical activity causing 50% lethality ($Ea-50$) of 0.058. It was also fitted to the PAH concentration in the PDMS, resulting in an $EC(PDMS)-50$ of 8.7 mM. Finally, the combined exposure to anthracene and pyrene was described by the sum of chemical activities causing lethality, in good agreement with the chemical activity-response curve obtained.
Using tree core samples to monitor natural attenuation and plume distribution

General information
State: Published
Organisations: Environmental Chemistry, Department of Environmental Engineering
Publication date: 2008
Peer-reviewed: Yes
Event: Abstract from ConSoil 3-6: The 10th international UFZ-Deltares/TNO conference on soil-water systems, Milano, Italy.
Electronic versions:
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Source: orbit
Source-ID: 220626
Research output: Research - peer-review » Conference abstract for conference – Annual report year: 2008

Degradation of PCB congeners by bacterial strains

General information
State: Published
Organisations: Department of Environmental Engineering, Helmholtz Centre for Environmental Research, Aarhus University
Contributors: Rein, A., Fernqvist, M., Mayer, P., Trapp, S., Bittens, M., Karlson, U.
Pages: 469-481
Publication date: 2007
Peer-reviewed: Yes

Publication information
Journal: Applied Microbiology and Biotechnology
Volume: 77
Issue number: 2
ISSN (Print): 0175-7598
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Determining Chemical Activity of (Semi)volatile Compounds by Headspace Solid-Phase Microextraction

This research introduces a new analytical methodology for measuring chemical activity of nonpolar (semi)volatile organic compounds in different sample matrices using automated solid-phase microextraction (SPME). The chemical activity of an analyte is known to determine its equilibrium concentration in the SPME fiber coating. On this basis, SPME was utilized for the analytical determination of chemical activity, fugacity, and freely dissolved concentration using these steps: (1) a sample is brought into a vial, (2) the SPME fiber is introduced into the headspace and equilibrated with the sample, (3) the SPME fiber is injected into the GC for thermal desorption and analysis, and (4) the method is calibrated by SPME above partitioning standards in methanol. Model substances were BTEX, naphthalene, and alkanes, which were measured in a variety of sample types: liquid polydimethylsiloxane (PDMS), wood, soil, and nonaqueous phase liquid (NAPL). Variable sample types (i.e., matrices) had no influence on sampling kinetics because diffusion through the headspace was rate limiting for the overall sampling process. Sampling time was 30 min, and relative standard deviations were generally below 5% for homogeneous solutions and somewhat higher for soil and NAPL. This type of activity measurement is fast, reliable, almost solvent free, and applicable for mixed-media sampling. © 2007 American Chemical Society.
Diffusion of PAH in potato and carrot slices and application for a potato model

A method for quantifying the effect of medium composition on the diffusive mass transfer of hydrophobic organic chemicals through thin layers was applied to plant tissue. The method employs two silicone disks, one serving as source and one as sink for a series of PAHs diffusing through thin layers of water, potato tissue, and carrot tissue. Naphthalene, phenanthrene, anthracene, and fluoranthene served as model substances. Their transfer from source to sink was measured by HPLC to determine a velocity rate constant proportional to the diffusive conductivity. The diffusive flux through the plant tissue was modeled using Fick's first law of diffusion. Both the experimental results and the model suggest that mass transfer through plant tissue occurs predominantly through pore water and that, therefore, the mass transfer ratio between plant tissue and water is independent of the hydrophobicity of the chemical. The findings of this study provide a convenient method to estimate the diffusion of nonvolatile organic chemicals through various plant materials. The application to a radial diffusion model suggests that "growth dilution" renders the concentration of highly hydrophobic chemicals in potatoes below their equilibrium partitioning level. This is in agreement with field results for the bioconcentration of PAHs in potatoes.

General information
State: Published
Organisations: Department of Environmental Engineering, Technical University of Denmark, Catholic University of the Sacred Heart, Aarhus University
Contributors: Trapp, S., Cammarano, A., Capri, E., Reichenberg, F., Mayer, P.
Pages: 3103-3108
Dynamic Permeation Method To Determine Partition Coefficients of Highly Hydrophobic Chemicals between Poly(dimethylsiloxane) and Water

Measurement of partition coefficients between poly(dimethylsiloxane) (PDMS) and water (K-PDMSw) becomes more and more difficult as the hydrophobicity of the compound increases. Experimental challenges include long extraction times, sorption to various surfaces and materials, and incomplete dissolution of the compound in the aqueous phase. In order to avoid these artifacts and to shorten experimental time, a dynamic permeation method was developed. According to steady-state diffusion theory, K-PDMSw is inversely proportional to the permeation rate through the aqueous boundary layer (ABL) from the donor PDMS to the acceptor PDMS. A simple ABL permeation reactor can thus be applied to determine K-PDMSw values of hydrophobic chemicals within a few days. The obtained values were in good agreement with those obtained using a conventional shaking method and the partition controlled delivery system. A good linear correlation was obtained between the logarithm of the 1-oc-tanol/water partition coefficient (log K-ow) from the literature and log K-PDMSw over 6 orders of magnitude.

General information
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Organisations: Swiss Federal Institute of Aquatic Science and Technology, Aarhus University
Contributors: Kwon, J., Wuethrich, T., Mayer, P., Escher, B. I.
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Journal: Analytical Chemistry
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.24
Web of Science (2017): Impact factor 6.042
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Effects of dilution on the exposure in sediment toxicity tests: Buffering of freely dissolved concentrations and changes in mixture composition

Some sediment toxicity tests, such as the Microtox test, are conducted by diluting either contaminated sediment or an aqueous phase with clean water. The present study aims to clarify how the dilution procedure affects the exposure of organisms. It is shown that freely dissolved concentrations of hydrophobic compounds are buffered by desorption from the sediment matrix when sediment is diluted with water. The buffering depends on the properties of the sediment matrix and contaminant. Consequently, the composition of a contaminant mixture changes with dilution, and the exposure in a sediment dilution toxicity test is poorly defined. This questions the application and subsequent assessments of such tests. Additionally, the often-observed higher toxicity in sediment dilution tests relative to elutriate dilution tests is not sufficient to claim direct contact exposure, because the enhanced sensitivity in sediment dilution tests also can be explained by buffering from the sediment matrix. In applying these tests, one should be aware of the fundamental differences between the sediment dilution strategy and the dilution of an aqueous phase and of the consequences it has for the outcome of the test.
Enhanced diffusion of polycyclic aromatic hydrocarbons in artificial and natural aqueous solutions

Uptake of hydrophobic organic compounds into organisms is often limited by the diffusive transport through a thin boundary layer. Therefore, a microscale diffusion technique was applied to determine the diffusive mass transfer of 12 polycyclic aromatic hydrocarbons through water, air, surfactant solutions, humic acid solutions, aqueous soil and horse manure extracts, digestive fluid of a deposit-feeding worm, and root exudates from willow plants. In most cases the diffusive mass transfer of PAHs was much higher through the tested media than through water, and the enhancement factors increased with increasing hydrophobicity of the PAHs. The diffusive flux of benzo[a]pyrene was for instance enhanced 74 times through gut fluid of a deposit-feeding worm when compared to water. These findings demonstrate that a wide variety of dissolved organic carbon (DOC) at environmental levels can enhance diffusive mass transfer in various transport scenarios. The diffusive uptake of PAHs into sediment dwelling organisms is particularly efficient within the gut and at direct contact with the sediment matrix. Bioremediation might be enhanced by the addition of auxiliary agents that enhance diffusive mass transfer. Enhanced diffusion needs also to be considered in dynamic transport models and for the operation and calibration of passive sampling techniques.

General information
State: Published
Organisations: Department of Environmental Engineering, Aarhus University, Roskilde University
Contributors: Mayer, P., Fernqvist, M., Christensen, P., Karlson, U., Trapp, S.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
Web of Science (2017): Impact factor 6.653
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
Web of Science (2016): Impact factor 6.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Web of Science (2015): Impact factor 5.393
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Web of Science (2012): Impact factor 5.257
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945
Web of Science (2011): Impact factor 5.228
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.979 SNIP 1.726
Web of Science (2010): Impact factor 4.827
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.86 SNIP 1.809
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.96 SNIP 1.935
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.774 SNIP 1.914
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.55 SNIP 1.893
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.608 SNIP 1.999
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.86 SNIP 2.046
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.54 SNIP 2.065
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.392 SNIP 1.949
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.387 SNIP 1.968
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 3.03 SNIP 2.315
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 3.367 SNIP 2.351
Equilibrium Sampling Through Membranes (ESTM) in hollow fibers combined with direct absorbance measurements

General information
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Organisations: Aarhus University
Contributors: Toräng, L., Larsson, N., Jonsson, J. Å., Mayer, P.
Publication date: 2007
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 15567
Research output: Research › Poster – Annual report year: 2007

Jämviktsprovtagning
Jämviktsprovtagning genom membran är ett nytt koncept där porösa hålfibrer används för upprening, anrikning och mätning av polära organiska föreningar och metaller. Metoden kan användas såväl i laboratoriet som till fältprovtagning

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State: Published
Organisations: Lund University, Aarhus University
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Peer-reviewed: Yes

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Journal: Kemivaerlden, Biotech, Kemisk Tidskrift
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Ratings:
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ISI indexed (2012): ISI indexed no
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Original language: Swedish
Research output: Research - peer-review › Journal article – Annual report year: 2007

Ligevægtsopsamling gennem membraner

General information
State: Published
Organisations: Danmarks Miljøundersøgelser, Lund University, Chinese Academy of Sciences
Contributors: Toräng, L., Reichenberg, F., Larsson, N., Liu, J., Romero, R., Jönsson, J. Å., Mayer, P.
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Peer-reviewed: Yes

Publication information
Journal: Dansk Kemi
Volume: 88
Issue number: 1
ISSN (Print): 0011-6335
Ratings:
ISI indexed (2013): ISI indexed no
Passive extraction and clean-up of phenoxy acid herbicides in samples from a groundwater plume using hollow fiber supported liquid membranes

Hollow fiber supported liquid membranes were applied for the passive extraction of phenoxy acid herbicides from water samples. Polypropylene hollow fiber membranes (240 μm i.d., 30 μm wall thickness, 0.05 μm pore size, 30 cm length) were impregnated with 2.0% tri-n-octylphosphine oxide (TOPO) in di-n-hexyl ether in the pores of the fiber wall to form a liquid membrane. They were then filled with basic solution in the lumen as acceptor and finally placed into the sample (donor). Complete extraction of phenoxy acid herbicides including 2,4-D, MCPA, dichlorprop, and mecoprop from an acidified sample (4 mL, adjusted to pH 1.5 with HCl) into basic acceptor (10 μL of 0.2 M NaOH) was achieved after 4 h of shaking (100 rpm) resulting in an enrichment factor of 400 times. The acceptor was then neutralized by addition of HCl and injected into a HPLC system for the determination of the phenoxy acid herbicides. Environmentally relevant salinity (0-3.5% NaCl) and dissolved organic matter (0-25 mg/L of dissolved organic carbon) had no significant effect on the extraction. The method provided extraction efficiencies of more than 91%, detection limits of 0.3-0.6 μg/L, and combined extraction and clean up in one single step. This procedure was applied to determine aqueous concentrations of phenoxy acid herbicides in groundwater samples collected from an old dumping site (Cheminova, Denmark) with detected concentrations up to 5800 μg/L. Although the samples were very dirty with large amounts of suspended particles, non-aqueous phase liquids (NAPLs) and dissolved organic matters, good spike recoveries (80-126%) were obtained for 10 of the 11 samples. (c) 2007 Elsevier B.V. All rights reserved.
Using solid phase microextraction to measure freely dissolved concentrations and chemical activities of PAHs in sediment cores of the western Baltic Sea

General information
State: Published
Organisations: Leibniz Institute for Baltic Sea Research Warnemunde (IOW), Aarhus University
Contributors: Witt, G., Liehr, G. A., Borck, D., Mayer, P.
Publication date: 2007
Peer-reviewed: No
Event: Poster session presented at SETAC Europe 17th Annual Meeting: Multiple stressors for the environment and human health - present and future challenges and perspectives, Porto, Portugal, 20-24 May,
Can Highly Hydrophobic Organic Substances Cause Aquatic Baseline Toxicity and can they Contribute to Mixture Toxicity?

Effect concentrations for aquatic baseline toxicity generally decrease with increasing log octanol-water partition coefficient (K-ow) values of up to 5 to 6, whereas less is known about the baseline toxicity of organic chemicals with log K-ow values above 6. A physicochemical analysis of the dissolution process for organic chemicals was combined with reported baseline toxicity data, leading to the following conclusions. First, no absolute hydrophobicity cutoff exists for baseline toxicity at a log K-ow value of 6, because aquatic baseline toxicity for fish and algae was observed for chemicals with log K-ow values greater than 6.5 and with effect concentrations less than 10 μg/L. Second, the baseline toxicity of hydrophobic organic substances was exerted at a relatively constant chemical activity of 0.01 to 0.1. Finally, organic chemicals with high melting points cannot provide sufficient chemical activity to exert baseline toxicity when considered as individual, pure chemicals. However, such substances are still expected to contribute to baseline toxicity when part of a complex mixture.

General information
State: Published
Organisations: Danish Centre for Environment and Energy
Contributors: Mayer, P., Reichenberg, F.
Pages: 2639-2644
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Environmental Toxicology and Chemistry
Volume: 25
Issue number: 10
ISSN (Print): 0730-7268
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.87 SJR 1.178 SNIP 1.018
Web of Science (2017): Impact factor 3.179
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.74 SJR 1.231 SNIP 1.021
Web of Science (2016): Impact factor 2.951
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3 SJR 1.433 SNIP 1.056
Web of Science (2015): Impact factor 2.763
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 2.89 SJR 1.501 SNIP 1.12
Web of Science (2014): Impact factor 3.225
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 2.88 SJR 1.656 SNIP 1.086
Web of Science (2013): Impact factor 2.826
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 2.81 SJR 1.639 SNIP 1.108
Web of Science (2012): Impact factor 2.618
ISI indexed (2012): ISI indexed yes
Continuous sampling of polar organic pollutants using commercially available hollow fibre cartridges - ESTM technique

General information
State: Published
Organisations: Danish Centre for Environment and Energy
Publication date: 2006
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 13646
Research output: Research › Poster – Annual report year: 2006

Equilibrium Sampling of Freely Dissolved Alkylphenols into a Thin Film of 1-Octanol Supported on a Hollow Fiber Membrane
A new negligible depletion extraction procedure was proposed for equilibrium sampling of 4-tert-octylphenol (OP) and 4-nonylphenol (NP) into a thin film of 1-octanol supported on a hollow fiber membrane. This thin liquid film extraction
A technique was directed at the determination of (1) freely dissolved concentrations, (2) distribution coefficients to 1-octanol (D-ow), and (3) binding to dissolved organic matter (D-DOC). The sampling device was prepared by dipping pieces of polypropylene microporous hollow fiber membrane (10-mm length, 30-μm wall thickness, 240-μm inner diameter) into 1-octanol for a few seconds to impregnate the pores of the hollow fiber wall. After stirring in 100 mL of sample solution for 24 h, the sampling device was harvested and desorbed with 30 μL of methanol, of which 20 μL was injected for HPLC analysis. With the measured Dow of a chemical and its equilibrium concentration in the 1-octanol sampling phase (C-octanol), the freely dissolved concentration (C-free) was calibrated based on C-free = C-octanol/D-ow. Measured log D-ow values of OP (4.32 +/- 0.06) and NP (4.79 +/- 0.02) were independent of the chemical concentration, only minimally affected by the environmentally relevant pH, buffering capacity, and salinity of samples, and agreed well with reported values. Log D-DOC values of OP (4.89 +/- 0.43) and NP (5.14 +/- 0.37), determined in Aldrich humic acid solution, agreed with reported partition coefficients to organic carbon (log K-oc) for particles in river water and effluent wastewater. Short equilibration times and high enrichment factors were obtained for both analytes due to the high surface to volume ratio of the new sampler. The technique was successfully applied to determine C-free of OP and NP in real water samples and to study their association with humic acids and bovine albumin.

General information
State: Published
Organisations: Chinese Academy of Sciences, Lund University, Danish Centre for Environment and Energy
Pages: 8526-8534
Publication date: 2006
Peer-reviewed: Yes

Publication information
Journal: Analytical Chemistry
Volume: 78
Issue number: 24
ISSN (Print): 0003-2700
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.24
Web of Science (2017): Impact factor 6.042
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.08
Web of Science (2016): Impact factor 6.32
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6
Web of Science (2015): Impact factor 5.886
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.79
Web of Science (2014): Impact factor 5.636
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.01
Web of Science (2013): Impact factor 5.825
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.8
Web of Science (2012): Impact factor 5.695
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.86
Web of Science (2011): Impact factor 5.856
Equilibrium Sampling Through Membrans (ESTM) in hollow fibers combined with direct absorbance measurements

General information
State: Published
Organisations: Danish Centre for Environment and Energy
Contributors: Toräng, L., Jonsson, J., Mayer, P.
Publication date: 2006
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 14903
Research output: Research › Poster – Annual report year: 2006

Measurement of accessibility and chemical activity of PAHs in polluted soil

General information
State: Published
Organisations: Danish Centre for Environment and Energy
Contributors: Reichenberg, F., Karlson, U., Mayer, P.
Publication date: 2006
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 14904
Research output: Research › Poster – Annual report year: 2006

Measuring the chemical activity of hydrophobic compounds by equilibrium sampling into silicone hollow fibers

General information
State: Published
Organisations: Danish Centre for Environment and Energy
Contributors: Toräng, L., Reichenberg, F., Glaesner, N., Mayer, P.
Publication date: 2006
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 14902
Research output: Research › Poster – Annual report year: 2006
Two Complementary Sides of Bioavailability: Accessibility and Chemical Activity of Organic Contaminants in Sediments and Soils

Research during the last decade has led to several competing concepts of bioavailability and to many more methods to measure bioavailability. One reason for disagreement is the confusion of two fundamentally different parameters, accessible quantity and chemical activity. The accessible quantity describes a mass of contaminants, which can become available to, for example, biodegradation and biouptake. It can be determined with mild extraction schemes or depletive sampling techniques. The chemical activity, on the other hand, quantifies the potential for spontaneous physicochemical processes, such as diffusion, sorption, and partitioning. For instance, the chemical activity of a sediment contaminant determines its equilibrium partitioning concentration in sediment-dwelling organisms, and differences in chemical activity determine the direction and extent of diffusion between environmental compartments. Chemical activity can be measured with equilibrium sampling devices and, theoretically, is closely linked to fugacity and freely dissolved concentration. The distinction between accessibility and chemical activity is outlined, and the benefits and limitation of both endpoints are provided. Finally, examples of how to measure and apply them are presented.
Effective chemical activity (EA50) used as a measure of exposure for baseline toxicity

General information
Equilibrium Sampling through Membranes of Freely Dissolved Chlorophenols in Water Samples with Hollow Fiber Supported Liquid Membrane

The freely dissolved concentration (C-free) of pollutants is generally believed to be bioavailable and thus responsible for toxic effects. The C-free of organic weak acids and bases consists of a dissociated and a nondissociated fraction. By using chlorophenols as model compounds, a negligible-depletion extraction technique, equilibrium sampling through membranes (ESTM), was developed for the measurement of the nondissociated part of the C-free. Polypropylene hollow fiber membranes (280-μm i.d., 50-μm wall thickness, 0.1-μm pore size, 15-cm length) were impregnated with undecane in the pores in the fiber wall as liquid membrane and filled with buffer solution in the lumen as acceptor. Then, the hollow fiber membranes were placed into the sample (donor) for an equilibrium extraction after sealing the two ends. The chlorophenol concentrations in the acceptor were then determined by direct injection into a HPLC system. Finally, the C-free of the nondissociated and the dissociated species of a chlorophenol were calculated based on its measured concentration in the acceptor, its pK(a) value, and the measured pH in sample and acceptor. Theoretically calculated distribution coefficients (D = 8-970) agree well with the experimental enrichment factors (E-e(max) = 6-1124), and the equilibration time was observed to increase with increasing distribution coefficients (hours to days). The freely dissolved concentration of five chlorophenols, with a wide range of pKa (4.9-9.2) and log K-OW (2.35-5.24), were successfully determined in model solutions of humic acids and at low-ppb levels in river and leachate water.
Equilibrium Sampling through Membranes of Freely Dissolved Copper Concentrations with Selective Hollow Fiber Membranes and the Spectrophotometric Detection of a Metal Stripping Agent

A sensitive spectrophotometric method for the determination of freely dissolved copper concentrations in aqueous samples after preconcentration with hollow fiber membrane extraction has been developed. The method is based on the equilibrium sampling through a selective membrane into an acceptor solution containing 4-(pyridyl-2-azo)resorcinol (PAR), which serves as stripping agent and metal indicator. Negligible extraction of interferences and equilibrium enrichment of copper allowed for selective spectrophotometric determination of the Cu-PAR complex. Some important extraction parameters such as acceptor composition, shaking, equilibrium time, and sample volume were studied. The optimized methodology showed good linearity in the range of 5-100 µg/L, an enrichment factor of 93, good repeatability and reproducibility (RSDs < 6%, n = 6), and a detection limit of 4 µg/L. The cationic metals Ni2+, CO2+, Cd2+, Fe3+, Pb2+, Zn2+, and Mn2+ were shown not to interfere with the measurement of Cu2+. Measurements on samples containing mixtures of various ligands and cations were in good agreement with theoretically calculated concentrations, and the method was also applied to environmental samples. The developed technique requires less labor and less sophisticated equipment than conventional methods typically based on atomic absorption spectrometry or ICP.

General information
State: Published
Organisations: Lund University, Danish Centre for Environment and Energy
Contributors: Romero, R., Liu, J., Mayer, P., Jönsson, J. Å.
Pages: 7605-7611
Publication date: 2005
Peer-reviewed: Yes

Publication information
Journal: Analytical Chemistry
Volume: 77
Issue number: 23
ISSN (Print): 0003-2700
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.24
Web of Science (2017): Impact factor 6.042
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.08
Web of Science (2016): Impact factor 6.32
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6
Web of Science (2015): Impact factor 5.886
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.79
Web of Science (2014): Impact factor 5.636
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.01
Web of Science (2013): Impact factor 5.825
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.8
Web of Science (2012): Impact factor 5.695
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.86
Web of Science (2011): Impact factor 5.856
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Impact factor 5.874
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2000): Indexed yes
Original language: English
DOI: 10.1021/ac050763a
Research output: Research - peer-review › Journal article – Annual report year: 2005
Quantifying the effect of medium composition on the diffusive mass transfer of hydrophobic organic chemicals through unstirred boundary layers

Unstirred boundary layers (UBLs) often act as a bottleneck for the diffusive transport of hydrophobic organic compounds (HOCs) in the environment. Therefore, a microscale technique was developed for quantifying mass transfer through a 100-μm thin UBL, with the medium composition of the UBL as the controllable factor. The model compound fluoranthene had to (1) partition from a contaminated silicone disk (source) into the medium, (2) then diffuse through 100 μm of medium (UBL), and finally (3) partition into a clean silicone layer (sink). The diffusive mass transfer from source to sink was monitored over time by measuring the fluoranthene content of the source and sink disks. The diffusive flux of fluoranthene was slightly higher for air than for water. Cyclodextrin, humic acids, and micelles of sodium dodecyl sulfate (SDS) enhanced the diffusive flux of fluoranthene in water by more than 1 order of magnitude. These results demonstrate that medium constituents, which normally are believed to bind hydrophobic organic chemicals, actually can enhance the diffusive mass transfer of HOCs in the vicinity of a diffusion source (e.g., contaminated soil particles). The technique can be used to evaluate the effect of natural fluids on diffusive mass transfer, as it integrates the different processes, partitioning and diffusion, in one laboratory model.
Sediment Dilution Method to Determine Sorption Coefficients of Hydrophobic Organic Chemicals

Sorption coefficients of hydrophobic organic chemicals (HOC) to sediments and soils can easily be underestimated in traditional batch experiments, especially because analysis of the aqueous concentration often includes compounds sorbed to colloidal organic matter. In this work, a "sediment dilution approach" has been combined with measurements of freely dissolved concentrations to determine sorption coefficients of five chlorobenzenes and two chloroanilines in spiked sediment and of two unknown chemicals in field-contaminated sediment. A range of sediment suspensions with different sediment-water ratios was made. Freely dissolved concentrations in these suspensions were measured by negligible depletion solid-phase microextraction (nd-SPME). Sediment-water sorption coefficients NO were derived from the

1.0.1021/es050556s
Source: orbit
Source-ID: 182061
Research output: Research - peer-review › Journal article – Annual report year: 2005
decrease of the freely dissolved concentrations as a function of the "dilution factor" (OF = volume water/mass sediment). The determined sorption coefficients were very similar to literature values. The experimental setup provides sorption coefficients without the need for total extractions, and the negligible depletion SPME technique does not require phase separation. The proposed method might be an alternative for batch equilibrium experiments to determine sorption coefficients.

**General information**
State: Published
Organisations: Utrecht University, National Institute for Coastal and Marine Management, Danish Centre for Environment and Energy
Pages: 4220-4225
Publication date: 2005
Peer-reviewed: Yes

**Publication information**
Journal: Environmental Science & Technology
Volume: 39
Issue number: 11
ISSN (Print): 0013-936X
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.58 SJR 2.535 SNIP 1.941
Web of Science (2017): Impact factor 6.653
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.26 SJR 2.559 SNIP 1.902
Web of Science (2016): Impact factor 6.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.61 SJR 2.546 SNIP 1.838
Web of Science (2015): Impact factor 5.393
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.5 SJR 2.777 SNIP 2.003
Web of Science (2014): Impact factor 5.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.52 SJR 2.952 SNIP 2.102
Web of Science (2013): Impact factor 5.481
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.17 SJR 3.115 SNIP 2.043
Web of Science (2012): Impact factor 5.257
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.16 SJR 3.18 SNIP 1.945
Web of Science (2011): Impact factor 5.228
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.979 SNIP 1.726
Web of Science (2010): Impact factor 4.827
A micro-scale technique to determine diffusive mass transfer of hydrophobic organics through diffusive boundary layers (DBLs)

General information
State: Published
Organisations: Danish Centre for Environment and Energy
Contributors: Mayer, P., Christensen, P. S., Johnsen, A. R., Karlson, U.
Publication date: 2004
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 11351
Research output: Research › Poster – Annual report year: 2004

A new technique to determine the diffusive mass transfer of hydrophobic organic substances through diffusive boundary layers (DBLs)

General information
State: Published
Organisations: Aarhus University
Contributors: Mayer, P., Christensen, P. S., Johnsen, A. R., Karlson, U.
Publication date: 2004
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 10606
Research output: Research › Poster – Annual report year: 2004
**Distinguishing Between The Availability And The Activity Of Organic Chemicals**

**General information**
State: Published
Organisations: Aarhus University
Contributors: Reichenberg, F., Mayer, P.
Publication date: 2004
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 11355
Research output: Research › Poster – Annual report year: 2004

**Equilibrium Sampling through Membrane: Hollow Fiber Supported Liquid Membrane for Static Sampling of Freely Dissolved Chlorophenols in Water**

**General information**
State: Published
Organisations: Aarhus University
Contributors: Liu, J., Jönsson, J. Å., Larsson, N., Mayer, P., Toräng, L.
Publication date: 2004
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 11361
Research output: Research › Poster – Annual report year: 2004

**Equilibrium Sampling through Membranes: Oprensning og opkoncentrering af polære stoffer med hollow fibers**

**General information**
State: Published
Organisations: Danish Centre for Environment and Energy
Contributors: Toräng, L., Mayer, P., Jönsson, J. Å., Liu, J.
Publication date: 2004
Peer-reviewed: No
Event:
Source: DMU
Source-ID: 11391
Research output: Research › Poster – Annual report year: 2004

**Towards continuous exposure measurements of polar organic priority pollutants**

**General information**
State: Published
Organisations: Aarhus University
Contributors: Larsson, N., Jönsson, J. Å., Liu, J., Mayer, P., Toräng, L.
Publication date: 2004
Peer-reviewed: No
Event: Poster session presented at ExTech, Leipzig, Germany.
Source: DMU
Source-ID: 11360
Research output: Research › Poster – Annual report year: 2004

**Equilibrium Sampling Devices**
A major thrust of environmental science over the past four decades has been improved and more extensive monitoring of organic and metallic contaminants in environmental media. We now recognize that the release of concentrations inevitable results in finite, and usually detectable, concentrations in air, water, soils, sediments, and animal and plant biota. These concentrations may exert adverse effects on ecosystems and human health through multiple sources and pathways with variable and often poorly understood degradation routes and rates. For example, significant concentrations can be established in unexpected places, such as cold climates.

**General information**
State: Published
Measured Pore-Water Concentrations Make Equilibrium Partitioning Work: A Data Analysis

There is an increasing body of evidence that the bioaccumulation of sediment-associated hydrophobic organic compounds (HOCs) is strongly influenced by sequestration. At present, it is not known how equilibrium partitioning theory (EqP), the most commonly employed approach for describing sediment bioaccumulation can be applied to sediments with sequestered contaminants. In this paper, we present freely dissolved pore-water concentrations of HOCs. These data were employed to interpret sediment bioaccumulation and sequestration data in order to arrive at a process based evaluation of EqP. The data analysis suggests that sediment bioaccumulation of compounds up to log K-OW 7.5 in Tubificidae can be described as bioconcentration from pore-water. In addition, the pore-water concentrations of HOCs (4.5 < log K-OW < 7.5) are established by equilibrium partitioning between the rapidly desorbing HOCs fraction in the sediment and the pore-water. Taken together, these findings indicate that EqP is a conceptually correct representation of sediment bioaccumulation, provided that sequestration is accounted for. This implies that the risk assessment of sediment-associated HOCs can be significantly simplified: With a method at hand for measuring freely dissolved pore-water concentrations of HOCs, it appears that HOCs' body residues in sediment dwelling organisms can be estimated on the basis of concentrations in pore-water and bioconcentration factors.
SPME-Measurements of Freely Dissolved Concentration of Hydrophobic Organic Compounds in the Microtox Solid Phase Test

General information
State: Published
Organisations: Unknown
Contributors: Laak, T. T., Busser, F., Mayer, P., Klamer, J. C., Hermens, J. L. M. D.
Publication date: 2002
Peer-reviewed: No
Event: Poster session presented at SETAC Europe 12th Annual Meeting, Vienna, Austria.
Source: DMU
Source-ID: 7912
Research output: Research - poster - Annual report year: 2002

Algal growth inhibition test in filled, closed bottles for volatile and sorptive materials
Exposure concentrations of many hydrophobic substances are difficult to maintain in algal growth inhibition tests performed in open agitated flasks. This is partly because such compounds tend to volatilize from aqueous solution and partly because of sorption to the algal biomass as well as to the test container. A simple filled closed bottle test with low algal densities and bicarbonate enrichment is described here as an approach to minimize the loss of test material from solution. The algal medium was enriched with 300 mg NaHCO3/L, the pH was adjusted to 7.0 by addition of HCl, and the resulting dissolved CO2 concentration supported maximum algal growth rates without pH drift for algal densities up to 4 mg dry weight/L. Two-day toxicity tests with kerosene were performed with this new test design and compared with an open bottle test and with a closed bottle test with headspace. Exposure concentrations of the volatile fraction of kerosene decreased by 99% in the open test, by 77% in the closed flask test with headspace, and by 16% in the filled closed bottle test. Algal growth inhibition was observed at much lower additions of kerosene in the new test design because of the improved maintenance of a constant exposure.

General information
State: Published
Organisations: Department of Environmental Science and Engineering, Utrecht University
Pages: 2551-2556
Publication date: 2000
Peer-reviewed: Yes

Publication information
Journal: Environmental Toxicology and Chemistry
Volume: 19
Issue number: 10
ISSN (Print): 0730-7268
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Accumulation and toxicity of lipophilic organic chemicals in phytoplankton algae and Daphnia, and partitioning of such compounds between water, particulates, and third phases of colloid and dissolved organic material

General information
State: Published
Organisations: Department of Environmental Science and Engineering
Contributors: Nyholm, N., Justesen, K. B., Kusk, K. O., Mayer, P., Halling-Sørensen, B.
Pages: 39-48
Publication date: 1998

Host publication information
Title of host publication: Report 1997. Danish Centre for Ecotoxicological Research
Place of publication: Silkeborg
Publisher: NERI
Source: orbit
Source-ID: 171569
Research output: Research › Book chapter – Annual report year: 1998

Influence of growth conditions on the results obtained in algal toxicity testing

General information
State: Published
Organisations: Department of Environmental Science and Engineering
Contributors: Mayer, P., Frickmann, J., Nyholm, N.
Pages: 1091 - 1098
Publication date: 1998
Peer-reviewed: Yes

Publication information
Journal: Environmental Toxicology and Chemistry
Volume: 17
ISSN (Print): 0730-7268
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.87 SJR 1.176 SNIP 1.018
Web of Science (2017): Impact factor 3.179
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.74 SJR 1.231 SNIP 1.021
Web of Science (2016): Impact factor 2.951
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3 SJR 1.433 SNIP 1.056
Web of Science (2015): Impact factor 2.763
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Toxic cell concentrations of three polychlorinated biphenyl congeners in the green alga Selenastrum Capricornutum
A simple in vitro fluorescence method for biomass measurements in algal growth inhibition tests

General information
State: Published
Organisations: Department of Environmental Science and Engineering
Contributors: Mayer, P., Cuhel, R., Nyholm, N.
Pages: 2525 - 2531
Publication date: 1997
Peer-reviewed: Yes

Publication information
Journal: Water Research
Volume: 31
Issue number: 10
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.55 SJR 2.601 SNIP 2.358
Web of Science (2017): Impact factor 7.051
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.49 SJR 2.663 SNIP 2.563
Web of Science (2016): Impact factor 6.942
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6.63 SJR 2.665 SNIP 2.482
Web of Science (2015): Impact factor 5.991
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 6.13 SJR 2.946 SNIP 2.702
Web of Science (2014): Impact factor 5.528
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2

General information
State: Published
Organisations: Department of Environmental Science and Engineering
Contributors: Mayer, P., Nyholm, N.
Number of pages: 302
Publication date: 1997
Host publication information
Title of host publication: A simple in vitro fluorescence method for biomass measurements in algal growth inhibition tests. (Abstract No. PWP187)
Place of publication: Pensacola, FL
Publisher: Society of Environmental Toxicology and Chemistry
Source: orbit
Source-ID: 169737
Research output: Research - peer-review › Book chapter – Annual report year: 1997

Growth inhibition of green alga S. capricornutum related to critical body burdens of PAHs and PCBs. (Abstract No. PWA124)

General information
State: Published
Organisations: Department of Environmental Science and Engineering
Contributors: Mayer, P., Halling-Sørensen, B., Nyholm, N.
Number of pages: 252
Publication date: 1997

Host publication information
Title of host publication: Growth inhibition of green alga S. capricornutum related to critical body burdens of PAHs and PCBs. (Abstract No. PWA124)
Place of publication: Pensacola, FL
Publisher: Society of Environmental Toxicology and Chemistry
Source: orbit
Source-ID: 169738
Research output: Research - peer-review › Book chapter – Annual report year: 1997

Influence of growth conditions on the results obtained in algal toxicity tests. (Abstract No. PHA105)

General information
State: Published
Organisations: Department of Environmental Science and Engineering
Contributors: Mayer, P., Frickmann, J., Nyholm, N.
Number of pages: 325
Publication date: 1997

Host publication information
Title of host publication: Influence of growth conditions on the results obtained in algal toxicity tests. (Abstract No. PHA105)
Place of publication: Pensacola, FL
Publisher: Society of Environmental Toxicology and Chemistry
Source: orbit
Source-ID: 169739
Research output: Research - peer-review › Book chapter – Annual report year: 1997

Projects:

Mixture Effects in Biodegradation Testing of Aromatic and Aliphatic Hydrocarbons
Hammershøj, R. H., PhD Student, Department of Environmental Engineering
Mayer, P., Main Supervisor, Department of Environmental Engineering
Andersen, H. R., Supervisor, Department of Environmental Engineering
Birch, H., Supervisor, Department of Environmental Engineering
Samfinansieret - Andet
15/06/2016 → 13/12/2019
Award relations: Mixture Effects in Biodegradation Testing of Aromatic and Aliphatic Hydrocarbons
Project: PhD

Linking the exposure and effects of organic chemical mixtures to their equilibrium partitioning concentrations in lipids
Trac, N. L., PhD Student, Department of Environmental Engineering
Mayer, P., Main Supervisor, Department of Environmental Engineering
Nørgaard Schmidt, S., Supervisor, Department of Environmental Engineering
Institut stipendie (DTU)
01/09/2015 → 15/03/2019
Award relations: Linking the exposure and effects of organic chemical mixtures to their equilibrium partitioning concentrations in lipids
Project: PhD

The effect of sorption and dosing on the degradation of poorly water soluble substances in different environmental matrices using standard OECD guidelines
Shrestha, P., PhD Student, Department of Environmental Engineering
Mayer, P., Main Supervisor, Department of Environmental Engineering
Birch, H., Supervisor, Department of Environmental Engineering
Hennecke, D., Supervisor
Stipendie fra udlandet
01/01/2016 → 31/12/2018
Award relations: The effect of sorption and dosing on the degradation of poorly water soluble substances in different environmental matrices using standard OECD guidelines
Project: PhD

Micropollutants removal for hospital wastewater
Tang, K., PhD Student, Department of Environmental Engineering
Andersen, H. R., Main Supervisor, Department of Environmental Engineering
Mayer, P., Supervisor, Department of Environmental Engineering
McArdell, C. S., Examiner
Privatist
01/01/2015 → 18/04/2018
Award relations: Micropollutants removal for hospital wastewater
Project: PhD

Aquatic toxicity testing for hazard identification of engineered nanoparticles
Sørensen, S. N., PhD Student, Department of Environmental Engineering
Baun, A., Main Supervisor, Department of Environmental Engineering
Hansen, S. F., Supervisor, Department of Environmental Engineering
Lützhøft, H. H., Supervisor
Mayer, P., Examiner, Department of Environmental Engineering
Kühnel, D., Examiner
Palmqvist, A., Examiner
Institut stipendie (DTU) Samf.
01/04/2012 → 30/06/2016
Award relations: Aquatic toxicity testing for hazard identification of engineered nanoparticles
Project: PhD

Investigating the feasibility of phytoremediation and phytoscreening
Nielsen, M. A., PhD Student, Department of Environmental Engineering
Trapp, S., Main Supervisor, Department of Environmental Engineering
Broholm, M. M., Supervisor, Department of Environmental Engineering
Mayer, P., Supervisor, Department of Environmental Engineering
Kjeldsen, P., Examiner, Department of Environmental Engineering
Burken, J. G., Examiner
Larsen, M., Examiner, Department of Environmental Engineering
Institut stipendie (DTU) Samf.
01/06/2011 → 01/07/2015
Award relations: Investigating the feasibility of phytoremediation and phytoscreening
Project: PhD

Improving the exposure basis of toxicological research on persistent organic pollutants and their mixtures
Gilbert, D., PhD Student, National Food Institute
Mayer, P., Main Supervisor
Vinggaard, A. M., Supervisor, National Food Institute
Trapp, S., Examiner
Scheringer, M., Examiner
Bioaccumulation and toxicity of lipophilic chemical in algae, crustaceans and fish

Lipophilic Organic Chemicals, LOC's constitute an important group of concern pollutants. LOC’s may bioconcentrate and even bioaccumulate via food webs (mostly in terrestrial systems). The compounds may be toxic not only to directly exposed populations of organisms but also cause indirect poisoning of man and other predators at the top of the food chain. While well studied with respect to toxicity and accumulation in fish, surprisingly little information has hitherto been available for other types of organisms, and the sorptive behaviour in surface waters, where algae may constitute a significant particulate phase, is generally not known. Information on sorption is important, nevertheless, not only for assessing the exposure of aquatic organisms to bioavailable toxicants, but also for the purpose of assessing the general chemical fate of LOC’s. Sedimentation mediated by sinking algae is here an important transport process moving the LOC’s from the water column to the sediments which may act as an ultimate sink and concern compartment since with no or slow biodegradation under the prevailing anaerobic conditions, large LOC concentrations may build up in time. The project aimed at contributing to fill the knowledge gaps on ecotoxicity to other organisms than fish, and further to investigate in detail the mechanisms involved in sorption and toxicity to phytoplankton algae including looking at the basic dose concept. According to current practice in aquatic ecotoxicology, concentration (total or dissolved) is used as a dose surrogate, while the real dose defining toxic exposure may either be the sorbed or bioaccumulated amount per unit of biomass or be the bioavailable concentration in partitioning equilibrium with this internal dose or biomass burden.

Activities:

7th SETAC World Congress
Period: 6 Nov 2016 → 10 Nov 2016
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry
Documents:
SETAC-Orlando-Abstract-Book

Related event

7th SETAC World Congress: SETAC North America 37th Annual Meeting
06/11/2016 → 10/11/2016
Orlando, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

7th SETAC World Congress
Period: 6 Nov 2016 → 10 Nov 2016
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry
Developing a strategy to improve the environmental risk assessment of difficult to test multi-component substances

Period: 2 Nov 2016 → 4 Nov 2016
Philipp Mayer (Invited speaker)
Department of Environmental Engineering
Environmental Chemistry
Documents:
RIFM ECETOC WS RA of Multiconsituent Substances

Related event

RIFM/ECETOC Workshop
02/11/2016 → 04/11/2016
Kissimmee, United States
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

International Society of Exposure Science
Philipp Mayer (Invited speaker)
Department of Environmental Engineering
Environmental Chemistry

Related event

International Society of Exposure Science 2016: 26th Annual Meeting: Interdisciplinary Approaches to Health and the Environment
09/10/2016 → 13/10/2016
Utrecht, Netherlands
Activity: Talks and presentations › Conference presentations

International Society of Exposure Science 26th Annual Meeting - ISES2016
Philipp Mayer (Invited speaker)
Department of Environmental Engineering
Environmental Chemistry

Related event

International Society of Exposure Science 26th Annual Meeting - ISES2016
09/10/2016 → 13/10/2016
Utrecht, Netherlands
Activity: Talks and presentations › Conference presentations

Congressi Stefano Franscini
Period: 29 May 2016 → 3 Jun 2016
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry
Documents:
Sjoholm

Related event

Congressi Stefano Franscini
29/05/2016 → 03/06/2016
Ascona, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

SETAC Europe 26th Annual Meeting
Period: 22 May 2016 → 26 May 2016
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry

**Related event**

**SETAC Europe 26th Annual Meeting: Environmental contaminants from land to sea: continuities and interface in environmental toxicology and chemistry**
Period: 22/05/2016 → 26/05/2016
Nantes, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**SETAC Europe 26th Annual Meeting**
Period: 22 May 2016 → 26 May 2016
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry

**Related event**

**SETAC Europe 26th Annual Meeting: Environmental contaminants from land to sea: continuities and interface in environmental toxicology and chemistry**
Period: 22/05/2016 → 26/05/2016
Nantes, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**SETAC**
Period: 1 Nov 2015 → 5 Nov 2015
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry

**Description**
173 Equilibrium sampling for a thermodynamic assessment of contaminated sediments
Documents:
173 Equilibrium sampling for a thermodynamic assessment of contaminated sediments
SETAC-SLC-Abstract-Book

**Related event**

**SETAC: Society of Environmental Toxicology and Chemistry North America 36th Annual Meeting**
Period: 01/11/2015 → 05/11/2015
Salt Lake City, Utah, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**SETAC**
Period: 1 Nov 2015 → 5 Nov 2015
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry

**Description**
WP139 Sorptive capacities of lipids determined by passive dosing of non-polar organic chemicals
Documents:
WP139 Sorptive capacities of lipids determined by passive dosing of non-polar organic chemicals
SETAC-SLC-Abstract-Book
Hydrophobic organic contaminants (HOCs) reaching the aquatic environment are largely stored in sediments. The risk of contaminated sediments is challenging to assess since traditional exhaustive extraction methods yield total HOC concentrations, whereas freely dissolved concentrations (Cfree) govern diffusive uptake and partitioning. Equilibrium sampling of sediment was introduced 15 years ago to measure Cfree, and it has since developed into a straightforward, precise and sensitive approach for determining Cfree and other exposure parameters that allow for thermodynamic assessment of polluted sediments. Glass jars with µm-thin silicone coatings on the inner walls can be used for ex situ equilibration while a device housing several silicone-coated fibers can be used for in situ equilibration. In both cases, parallel sampling with varying silicone thicknesses can be applied to confirm valid equilibrium sampling (method incorporated QA/QC). The measured equilibrium concentrations in silicone (CSil) can then be divided by silicone/water partition ratios to yield Cfree. CSil can also be compared to CSil from silicone equilibrated with biota in order to determine the equilibrium status of the biota relative to the sediment. Furthermore, concentrations in lipid at thermodynamic equilibrium with sediment (Clip\textsubscript{Sed}) can be calculated via lipid/silicone partition ratios CSil × KLip:Sil, which has been done in studies with limnic, river and marine sediments. The data can then be compared to lipid-normalized concentrations in aquatic organisms or to regulatory thresholds. Finally, CSil can also be converted into chemical activities (a), which express the energetic level of the chemicals, drive several spontaneous processes and are well linked to the potential for baseline (mixture) toxicity. This overview lecture will focus at the latest developments in equilibrium sampling concepts and methods. Further, we will explain how these approaches can provide a new basis for a thermodynamic assessment of polluted sediments.

Links:
Around 70% of industrial chemicals are hydrophobic compounds which are assumed to elicit toxicity through narcosis by accumulating in membranes and disrupting membrane integrity and function. Although narcosis has been recognized as an important toxicity mechanism for decades, ecotoxicological research has been mostly limited to the development of quantitative structure activity relations (QSARs) to predict toxicity, resulting in insufficient understanding of the exact mechanisms involved. In this study we investigate specific aspects of the mechanism of narcosis in fish using both alternative in vivo (zebrafish embryo) and in vitro tests. We applied a passive dosing method to expose zebrafish embryos up to 5 days post fertilization to linear dilution series of a set of non-polar narcotics (phenanthrene and three chlorobenzene structure analogues). In addition to increasing mortality, we observed decreasing growth, heart rate and motility with increasing exposure concentration of all narcotics, consistent with the general assumption of reduced cardiorespiratory function. At the cellular level, the cell membrane is expected to be the first target of narcotics. Since the mitochondrial and endoplasmic reticulum membrane are known to closely interact with the cell membrane, we hypothesize that narcotics can be further partitioned into these organelle membranes where they can disrupt essential membrane-bound processes. The electron transport chain (ETC) is an example of a crucial mitochondrial membrane-bound process and is therefore a potential target. We found that in zebrafish embryos ETC activity was increased at low exposure concentrations, suggesting a compensatory response, while it decreased when exposure concentrations reached levels causing reduced motility, heart rate and eventually mortality. The effect of narcotic compounds on ETC activity was confirmed in vitro: we observed inhibition of the ETC after adding the compounds directly to a homogenate of control embryos. To further investigate effects on the energy production system, and to characterize the observed compensatory response, we are currently measuring the effect of narcotics on ATP synthase activity both in vivo and directly in vitro. Although narcosis is commonly considered a non-specific mechanism of toxicity acting by membrane disruption in general, we illustrate how we can increase our understanding of narcosis by focussing on specific membrane types and membrane-bound processes.

Related event

SETAC: Society of Environmental Toxicology and Chemistry North America 36th Annual Meeting
01/11/2015 → 05/11/2015
Salt Lake City, Utah, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

SETAC
Period: 1 Nov 2015 → 5 Nov 2015
Philipp Mayer (Participant)
Department of Environmental Engineering
Environmental Chemistry

Description
and Stine Nørregaard Schmidt
Poster
Authors: Stine Schmidt, James Armitage, Jon Arnot, Philipp Mayer
Titel: Linking algal growth inhibition to chemical activity
Unitless chemical activity, expressing the energetic level of a compound relative to its energetic level in pure liquid [0-1], has proven useful to quantify the effective exposure to hydrophobic organic compounds through both aerial and aqueous media. Several studies have linked toxicity to chemical activity, as opposed to e.g. the total concentration. Baseline toxicity (narcosis) for neutral hydrophobic organic compounds has been shown to initiate in the narrow chemical activity range of 0.01 to 0.1. This presentation focuses on linking algal growth inhibition to chemical activity with the aims to (1) further challenge the current chemical activity range for baseline toxicity, and (2) extend the utilisation of the chemical activity concept across compounds and species. The first part of the presentation focuses on results from a recently published study, in which toxicity data for 39 non-polar liquids were applied to challenge the chemical activity range for baseline toxicity. For each compound, the effective activity (Ea50) was estimated as the ratio of the effective concentration (EC50) and water solubility. Of these ratios, 90% were within the expected chemical activity range of 0.01 to 0.1. This presentation focuses on linking algal growth inhibition to chemical activity with the aims to (1) further challenge the current chemical activity range for baseline toxicity, and (2) extend the utilisation of the chemical activity concept across compounds and species. The first part of the presentation focuses on results from a recently published study, in which toxicity data for 39 non-polar liquids were applied to challenge the chemical activity range for baseline toxicity. For each compound, the effective activity (Ea50) was estimated as the ratio of the effective concentration (EC50) and water solubility. Of these ratios, 90% were within the expected chemical activity range of 0.01 to 0.1. On a practical level, these findings suggest EC50 values for baseline toxicity to be at or above 1% of water solubility. On an environmental risk assessment level, predicted no-effect concentrations (PNECs) for baseline toxicity could even be set as a percentage of saturation, and this approach can easily be extended to baseline toxicity of mixtures. However, EC50 values well below 1% of saturation can still occur and indicate the potential for excess toxicity through a specific or reactive mode of action. The second part of the presentation focuses on extending the utilisation of the chemical activity concept. More specifically, the chemical activity concept is applied to a much larger range of algal toxicity data, including a wide range of solids and liquids, covering several expected modes of action and also several algal species. High-quality toxicity data are carefully selected from peer-reviewed scientific literature and QSAR databases. This presentation shows how the chemical activity concept can be used to compare and combine toxicity data across compounds and species in order to characterize toxicity – and further how the concept can be used in environmental risk assessment.
Sorptive capacities of lipids determined by passive dosing of non-polar organic chemicals

Authors: Annika Jahnke, Amelie Kierkegaard, Damien Bolinius, Philipp Mayer, Jan Holmbäck, Matthew MacLeod

Lipids often are considered the major partitioning phase for non-polar organic chemicals. What is referred to as "lipid", however, is a complex matrix consisting of a highly variable mixture of neutral ("storage") and polar ("membrane") lipids that usually is operationally defined by the extraction protocol. Furthermore, depending on an organism's fraction of lipids and proteins and the properties of a chemical, other sorptive phases (e.g. proteins) may be particularly important. The aim of the present study was to expand our previous studies of the sorptive capacities of pure storage lipids into other pure phases and more realistic media, i.e. extractable organic matter (EOM) obtained by lipid extraction of various biota samples. Our experimental protocol included: i) extraction of biota tissues; ii) passive dosing of replicates of each EOM sample with cyclic volatile methylsiloxanes (cVMS), chlorobenzenes and polychlorinated biphenyls via a common headspace over an olive oil donor phase to transfer the same chemical activity into the samples; iii) sampling of EOM and olive oil controls at different time points; iv) purge-and-trap extraction of the model chemicals onto ENV+ SPE cartridges, elution and GC/MS analysis; v) characterization of the lipid composition in all samples via NMR. Our experiments demonstrate that the sorptive capacities of the EOM samples do not differ significantly from the olive oil controls if the EOM consists of neutral lipids only. However, the EOM samples show small but statistically significant differences in their sorptive capacities for the (semi)volatile model chemicals if other components such as phosphatidylcholine (PC) and cholesterol are present in quantifiable amounts. Based on the lipid composition quantified by NMR and literature data for the chemicals' partition ratios between PC/water and storage lipid/water, we modeled the chemicals' partitioning into the EOM and compared the model results to the measured concentrations. The study provides a new basis for unravelling biomagnification, since an increase in concentration with trophic level can be divided into a sorption capacity effect and an increase in chemical activity.

Related event

SETAC: Society of Environmental Toxicology and Chemistry North America 36th Annual Meeting
01/11/2015 → 05/11/2015
Salt Lake City, Utah, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Foundational aspects of the concept of chemical activity

Philipp Mayer (Lecturer)
Department of Environmental Engineering
Environmental Chemistry
Documents:
2015 Foundational aspects of the concept of chemical activity
Related event

ECETOC: Defining the role of chemical activity in environmental risk assessment within the context of mode of action: Practical guidance and advice
29/10/2015 → 30/10/2015
Snowbird Resort, Utah, United States
Activity: Talks and presentations › Conference presentations

Equilibrium Sampling of Hydrophobic Organic Contaminants in Sediment
Philipp Mayer (Lecturer)
Department of Environmental Engineering
Environmental Chemistry
Documents:
Short intro guide on How to use the VidyoRoom Video Conference System at ENV

Related event

250th American Chemical Society National Meeting
16/08/2015 → 20/08/2015
Boston, United States
Activity: Talks and presentations › Conference presentations

ICCA-LRI and JRC Workshop 2014
Period: 17 Jun 2014
Philipp Mayer (Invited speaker)
Department of Environmental Engineering
Environmental Chemistry

Description
Assessing toxicity with partitioning based methods and chemical activity.
Philipp Mayer.

Related event

ICCA-LRI and JRC Workshop 2014
17/06/2014 → 18/06/2014
Lugano, Switzerland
Activity: Talks and presentations › Conference presentations