

Equilibrium sampling for a thermodynamic assessment of contaminated sediments - DTU Orbit (08/11/2017)

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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_{free}) govern diffusive uptake and partitioning. Equilibrium sampling of sediment was introduced 15 years ago to measure C_{free} , and it has since developed into a straightforward, precise and sensitive approach for determining C_{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_{sil}) can then be divided by silicone/water partition ratios to yield C_{free} . C_{sil} can also be compared to C_{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 ($C_{lip?Sed}$) can be calculated via lipid/silicone partition ratios $C_{sil} \times K_{lip:sil}$, 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_{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, Stockholm University

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Number of pages: 1

Publication date: 2015

Event: Abstract from SETAC North America 36th Annual Meeting, Salt Lake City, UT, United States.

Main Research Area: Technical/natural sciences

Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015