Using equilibrium passive sampling for exposure assessment of hydrophobic organic chemicals in sediment

Summary Equilibrium passive sampling of sediments can yield a measure for freely dissolved and lipid based concentrations of hydrophobic organic chemicals (HOC). Hence, they provide an improved exposure basis for the risk assessment of HOC contaminated sediments.

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Principle of equilibrium passive sampling[1]

The concentrations of hydrophobic organic chemicals (HOCs) differ between environmental compartments due to differences in their capacity for HOCs. However, in equilibrium the ratio of concentration and capacity is equal for each compartment and consequently equal for an equilibrated passive sampler (Fig. 1). Hence, equilibrium passive samplers can act as a reference partitioning phase and as a tool to measure chemical activity.[2]

Of the compartments in Fig. 1, a passive sampler gives the most precise measure of the concentration-capacity ratio, since (1) its concentration is measured sensitively and precisely and (2) its capacity is well defined and constant. For all other compartments, either the concentration is analytically challenging to determine or they have a poorly defined or variable capacity.

Application for exposure assessment

After equilibration with the sediment (Box 1), the concentration in the sampler ($C_{Polymer}$) can be converted to equilibrium partitioning concentrations in other compartments with existing EQS (Fig. 2).

① $C_{Polymer}$ divided by the polymer–water partition coefficient ($K_{Polymer,W}$) provides the free dissolved concentration (C_W) in pore water.

② C_W is linked to concentrations in biota through the bioaccumulation factor (BAF) or bioconcentration (BCF).

③ Through the lipid–polymer partition coefficient[3] ($K_{Lipid,Polymer}$), $C_{Polymer}$ can be expressed as a lipid based concentration (C_{Lipid}). $K_{Lipid,Polymer}$ is almost identical for different lipids[3].

④ The C_W obtained in ② can also be converted to a lipid basis using the lipid–water partition coefficient ($K_{Lipid,W}$).

Biotic concentrations have a high natural variability and so have the BCF or BAF required in ②.

①,③ and ①+④ convert to a defined compartment, pure water or model lipid, using physical constants and consequently results represent a well defined exposure level.

Monitoring remediation

The C_W measured by passive sampling is a good indicator for progress of remediation. Application of a range of sampler-sediment ratios (Box 2) provides a release pattern indicating where remediation can progress.

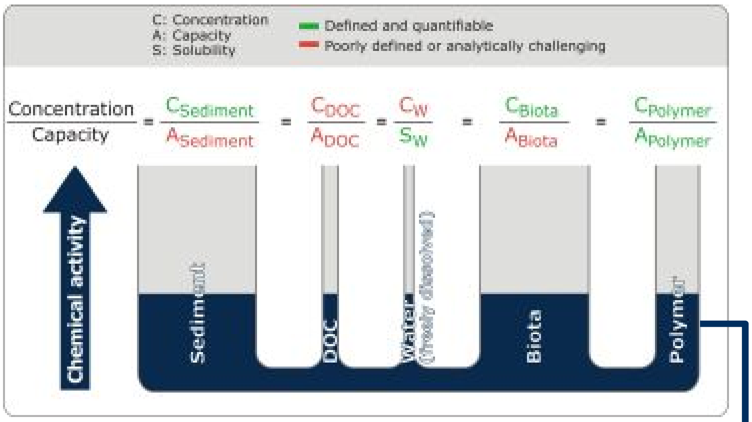


Fig. 1. The level of contamination is best expressed in a medium that (1) allows sensitive, precise concentration measurements and (2) provides a well defined, constant capacity. An equilibrated passive sampling polymer can provide this combination.

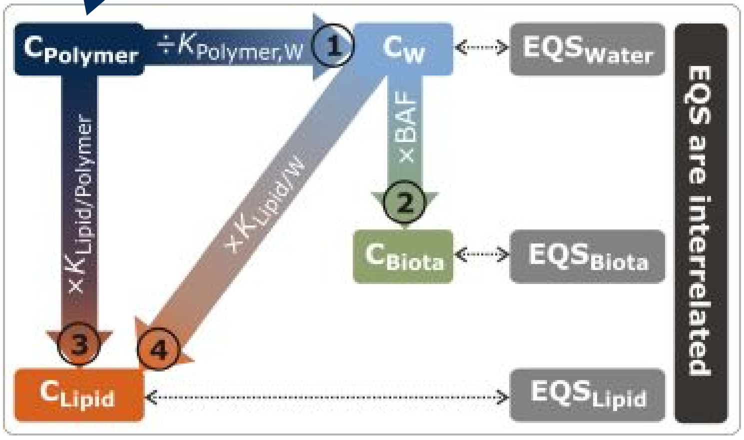
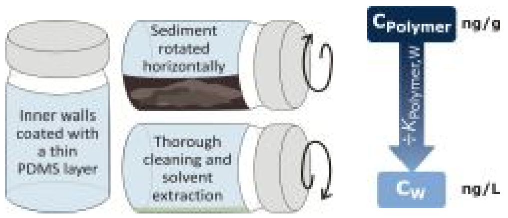


Fig. 2. Conversion of the concentration in the polymer to equilibrium partitioning concentrations in various compartments relevant for risk assessment.

Box 1: Non- depletive passive sampling of sediment

Polymer coated glass jars[4] with multiple coating thickness are equilibrated with excess sediment. From $C_{Polymer}$, C_W and C_{Lipid} are calculated by division or multiplication with appropriate partition coefficients (Fig. 2).



References

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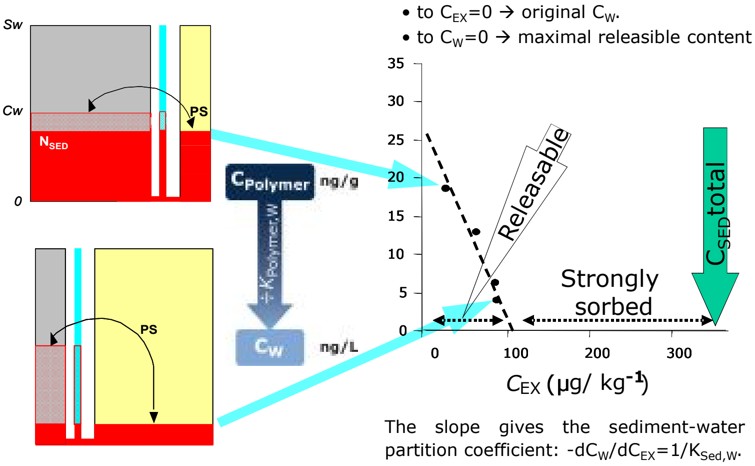
Box 2: Multi ratio passive sampling[5] of sediment – desorption isotherm

A passive sampler (PS) with a very low capacity will not deplete the sample → C_W remains constant.

A plot of C_W versus the extracted concentration (C_{EX}) allows two way extrapolation

- to C_{EX}=0 → original C_W.
- to C_W=0 → maximal releasible content



A PS with a high capacity will deplete the sample → C_W decreases.

The slope gives the sediment-water partition coefficient: $-dC_W/dC_{EX}=1/K_{Sed,W}$. Soxhlet extraction yields both the releasable and strongly sorbed fractions.