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Hexachlorobenzene

A concentration of 100 µg hexachlorobenzene (HCB) per kg wet weight has been measured in fish that live and in the sediment/water interface. The average fat content of the fish is about 5 % (i.e. 0.05 kg lipid per kg wet weight). The aqueous concentration of HCB in water was determined to be 0.1 ng L⁻¹, in the sediment ($f_{oc} = 0.05 \text{ kg}_{oc} \text{ kg}^{-1}$ in dry sediment) a concentration of 2 µg kg⁻¹ sediment (dry) was analysed.

Estimate (roughly) which concentration one would expect in the fish (in µg per kg wet weight) if they were in equilibrium with

- the water phase or
- the sediment phase.

What assumptions do you make?

Use the following partition constants:

$$\log K_{\text{lipid/water}} = 5.8 \text{ (L}_{\text{water}}/\text{L}_{\text{lipid}})$$

$$\log K_{\text{oc/water}} = 5.3 \text{ (L}_{\text{water}}/\text{kg}_{oc})$$

Answer:

a) 100 µg per kg wet weight correspond to $2 \cdot 10^6$ ng per kg lipid. In equilibrium with water one would expect $6.3 \cdot 10^4$ ng/kg_{lipid} if HCB only partitions into fish lipids.

On basis of the total wet weight of the fish one would expect a concentration of 3.15 µg/kg_{wet weight} instead of the 100 µg/kg_{wet weight} that have been measured.

b) The K_{oc} is $2 \cdot 10^5 \text{ L}_{\text{water}}/\text{kg}_{oc}$. The sediment/water partition constant thus is $1 \cdot 10^4 \text{ L}_{\text{water}}/\text{kg}_{\text{sediment}}$

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because only 5% of the sediment is organic carbon. The equilibrium concentration in the pore water then was about $2 \cdot 10^{-4} \mu\text{g} / \text{L}_{\text{water}}$ oder $0.2 \text{ ng} / \text{L}_{\text{water}}$ based on the measured $2 \mu\text{g kg}^{-1}$ in wet sediment. In equilibrium with the sediment one would expect $1.26 \cdot 10^5 \text{ ng/kg}_{\text{lipid}}$ if HCB only partitions into the fish lipids.

Conclusion: The fish cannot have been contaminated from either the water or the sediment phase. Most likely they have been contaminated via the food chain and the up-take kinetics with the food are so much faster than the clearance kinetic via the water phase that no equilibrium with water is achieved.

