Annex 4

Calculation of fugacity ratios

The log K_{ow} values for D4 and D5 are 6.49 and 8.03, respectively. If it is assumed that lipid partitioning is equal to octanol partitioning, the lipid-water partition coefficients for D4 and D5 become 3,090,000 and 107,000,000 L water/kg lipid, respectively (10^6.49 and 10^8.03).

The experimental organic carbon-water partition coefficients (K_{oc}) for D4 and D5 are 17,000 and 150,000 L water/kg oc, respectively.

The fugacity ratio will be one if lipid and organic carbon are in equilibrium with each other via the pore water phase. This will be at a biota-to-sediment-accumulation-factor (BSAF in kg lipid/k oc) that is equal to the ratio of the lipid-water partition coefficient (which is equal to K_{ow}) and the organic carbon-water partition coefficients (i.e. by calculating the concentration in lipids and organic carbon, using the same pore water concentrations).

These BSAF values will be 3,090,000/17,000=180 for D4 and 107,000,000/150,000=710 for D5. These values are extraordinarily high and are strongly dependent on the assumptions that partitioning to lipids is equal to partitioning to octanol, while using experimental values for K_{oc} at the same time.

If for example the Karickhoff equation for K_{oc} is used instead (log K_{oc}= log K_{ow} -0.21; cf. ECHA guidance on IR and CSA R11, p 118), it would follow that a BSAF of 1.6 would correspond to a fugacity ratio of one.