Supporting Information

Partitioning based dosing – an approach to include bioavailability in the effect directed analysis of contaminated sediment samples

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GC-MS

For liquid samples an Agilent 7683 Series Autosampler (Böblingen, Germany) was used. The carrier gas was helium at a constant flow of 1.3 mL/min. 1 µL of the sample was injected using pulsed splitless mode at 250 °C. The following oven program was used: 60 °C to 150 °C with a rate of 30 °C/min, 150 °C to 186 °C with a rate of 6 °C/min and from 186 °C to 280 °C with a heating rate of 4 °C/min. The final temperature of 280 °C was held for 7 min. The mass selective detector was operated either in SCAN mode or in selective ion monitoring mode (SIM).

The loaded SPME-fibres were desorbed in the inlet of the GC-MS for five minutes in the splitless mode at 270 °C (DVB/CAR/PDMS fibre) and 300 °C (PA), respectively. The carrier gas was helium at a constant flow of 1.3 mL/min. The oven was heated from 60 °C to 280 °C with a rate of 120 °C/min, to the final temperature of 280 °C, which was held for seven minutes. Solid phase microextraction based analysis was calibrated with external standards dissolved in methanol and diluted with GB-medium to 0.1 % solvent content. In order to avoid any disturbing of equilibration processes non-depletive extraction in the kinetic phase for 5 min at a stirring velocity of 200 r.p.m. and a temperature of 28 °C was applied. For all standard compounds (see table S1) extracted fractions remained below 7.5 %, which was taken as a criterion for non-depletive extraction.

Table S1: Model substances and their physico-chemical properties.

Chemical	CAS number	Log K_{OW}*	Solubility* in water (mg/L)	Supplier
methyl-parathion	298-00-0	2.80	37.7	Riedel de Haen
promethryn	7287-19-6	3.51	33.0	Riedel de Haen
anthraquinone	84-65-1	3.39	1.35	Fluka
lindane	58-89-9	3.72	7.3	Riedel de Haen
N-phenyl-2-naphthylamine	135-88-6	4.40	6.31	Aldrich
pyrene	129-00-0	4.88	0.135	Merck
methoxychlor	72-43-5	5.08	0.1	Riedel de Haen
fluoranthene	206-44-0	5.16	0.26	Riedel de Haen
benz[*a*]anthracene	56-55-3	5.76	0.0094	Fluka
p,p'-DDD	72-54-8	6.02	0.09	Riedel de Haen
PCB 101	35065-28-2	6.22	0.0154	Promochem

* Epi Suite v.3.20, 2007, U.S. Environmental Protection Agency.

The chemicals were chosen to cover a broad range of K_{OW} and different chemical structures. All compounds have been identified as relevant toxicants in previous studies on sediments from Bitterfeld (1), which were selected as one of the cases in the present study.

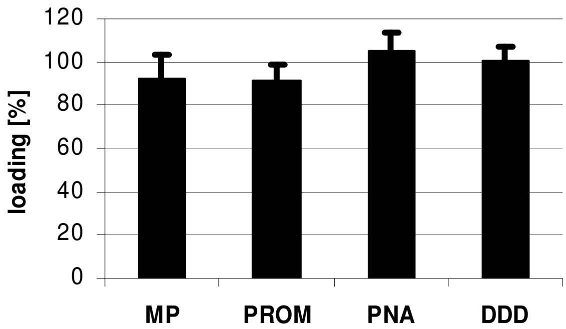

Figure S1: Loading efficiency in percent (n = 3) of methyl-parathion (MP), prometryn (PROM), N-phenyl-2-naphthylamine (PNA) and p,p'-DDD on SRs.

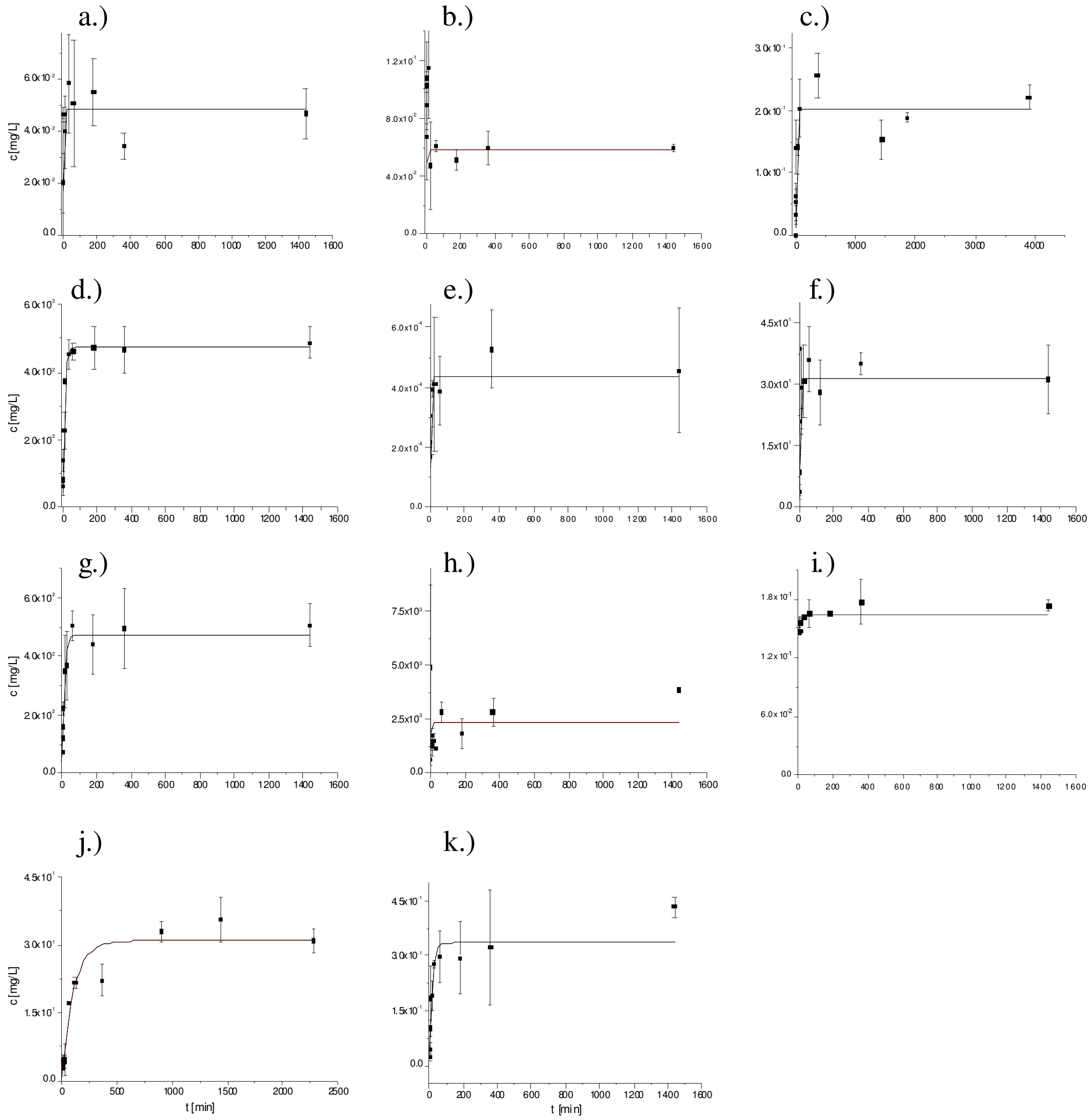

Figure S2: Depletion kinetics from SRs into the aqueous phase a.) *p,p'*-DDD, b.) fluoranthene, c.) prometryn, d.) pyrene, e.) benzo[*a*]anthracene, f.) anthraquinone, g.) methoxychlor, h.) PCB 101, i.) methyl-parathion j.) lindane k.) N-phenyl-2-naphthylamine.

REFERENCES

(1) Brack, W.; Altenburger, R.; Ensenbach, U.; Möder, M.; Segner, H.; Schüürmann, G. Bioassay-directed identification of organic toxicants in river sediment in the industrial region of Bitterfeld (Germany) - A contribution to hazard assessment. *Arch. Environ. Contam. Toxicol.* **1999,** *37*, 164-174.