Experimental verification of a model describing solid phase microextraction (SPME) of freely dissolved organic pollutants in sediment porewater

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ABSTRACT
To verify a theoretical mass balance and multiple compartment partitioning model developed to predict freely dissolved concentrations (FDCs) of hydrophobic organic chemicals (HOCs) using negligible depletion- solid phase microextraction (nd-SPME), a series of sediment slurry experiments were performed using disposable poly(dimethyl)siloxane (PDMS) coated-SPME fibers and 14C-radiolabeled HOC analogs. First, pre-calibration of disposable PDMS coated fibers for four model compounds (phenanthrene, PCB 52, PCB 153 and p,p'-DDE) with good precision (<10%) was achieved. Second, sediment slurries spiked and aged with the radiolabeled analogs were extracted by SPME with manipulation of the sediment slurry mass (m_s) or the PDMS coating volume (V_f). The measured extent of depletion by SPME (x_e) decreased with increasing sediment mass (m_s); conversely, x_e increased with increasing V_f, which is consistent with the theoretical prediction from our previous model [Yang, Z.-Y., Zeng, E.Y., Maruya, K.A., Mai, B.-X., Ran, Y., 2007. Predicting organic contaminant concentrations in sediment porewater using solid-phase microextraction. Chemosphere 66, 1408–1414]. Moreover, the SPME-measured FDCs (C_{pw,SPME}) followed the order of phenanthrene > PCB 52 > PCB 153, and the measured and predicted C_{pw} values were not substantially different from empirically determined values except for p,p'-DDE.

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