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## **A two-component mass balance model for calibration of solid-phase microextraction fibers for pyrethroids in seawater**

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### **ABSTRACT**

Determination of the analyte-specific distribution coefficient between the aqueous and sorbing phases is required for estimation of the aqueous-phase concentration of the analyte of interest using polymeric materials. Poly(dimethylsiloxane)-coated solid-phase microextraction (PDMS-SPME) fiber-water partition coefficient ( $K_f$ ) values for eight common-use pyrethroids were determined using a two-compartment mass balance model and parameters determined in experimental seawater microcosms. Mass balance, epimerization, and aqueous-phase degradation (i.e., hydrolysis) were characterized using gas chromatography-negative chemical ionization mass spectrometry to facilitate  $K_f$  estimation. Of the eight pyrethroids, only bifenthrin exhibited increasing sorption on the SPME fiber over the entire time-series exposure, indicating that its  $K_f$  value could be estimated through a stable-compound model. The remaining pyrethroids were found to be unstable (half-life of <22 days), underscoring the importance of accounting for degradation in estimating  $K_f$ . The two-compartment model explained the experimental time-series data for bifenthrin ( $R^2 > 0.98$ ) and the remaining unstable pyrethroids ( $R^2 > 0.7$ ), leading to estimated values of  $\log K_f$  between 5.7 and 6.4, after correcting for residual dissolved organic carbon (DOC) in the experimental seawater. These  $K_f$  values can be used to determine freely dissolved pyrethroid concentrations in the pg/L range using PDMS-SPME in fresh or seawater matrices under equilibrium conditions in laboratory or field applications.

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