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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 coefficients (K_f s) 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 timeseries 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 <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 to 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.

Full Text

http://ftp.sccwrp.org/pub/download/DOCUMENTS/AnnualReports/2012AnnualReport/ar12_085_098.pdf