SCCWRP #1044

An exponential model based new approach for correcting aqueous concentrations of hydrophobic organic chemicals measured by polyethylene passive samplers

Wenjian Lao[1], Keith A. Maruya[1], David Tsukada[2]

[1]Southern California Coastal Water Research Project, Costa Mesa, CA, USA
[2]Retired

ABSTRACT

Although low density polyethylene (PE) passive samplers show promise for the measurement of aqueous phase hydrophobic organic chemicals (HOCs), the lack of a practical and unsophisticated approach to account for non-equilibrium exposure conditions has impeded widespread acceptance and thus application in situ. The goal of this study was to develop a streamlined approach based on an exponential model and a convection mass transfer principle for correcting aqueous concentrations for HOCs deduced by PE samplers under non-equilibrium conditions. First, uptake rate constants ($k1$), elimination rate constants (k_2), and seawater-PE equilibrium partition coefficients (KPEWs) were determined in laboratory experiments for a diverse suite of HOCs with $logK_{ow}$ range of 3.4–8.3. Linear relationships between log $k2$ and $logK_{ow}$, and between log KPEW and $logK_{ow}$ were established. Second, PE samplers pre-loaded with 13C-labeled performance reference compounds (PRCs) were deployed in the ocean to determine their $k2$ in situ. By applying boundary layer and convection mass transfer theories, ratio (C) of $k2$ values in field and laboratory exposures was estimated. This C value was demonstrated a constant that was only determined by water velocities and widths of PE strips. A generic equation with C and $logK_{ow}$ as parameters was eventually established for extrapolation of non-equilibrium correction factors for the water boundary layer-controlled HOCs. Characterizing the hydrodynamic conditions indicated the sampler configuration and mooring mode should aim at sustaining laminar flow on the PE surface for optimal mass transfer. The PE estimates corrected using this novel approach possessed high accuracy and acceptable precision, and can be suited for a broad spectrum of HOCs. The presented method should facilitate routine utilization of the PE samplers..