

**Title:** Using Performance Reference Compounds (PRCs) to measure dissolved water concentrations ( $C_{\text{free}}$ ) in the water column: Assessing equilibrium models

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**Track and Session:**

**Keywords:** passive sampling; performance reference compounds; PCBs; equilibrium

**Preference:** Platform

**Abstract:**

Equilibrium-based passive sampling methods are often used in aquatic environmental monitoring to measure hydrophobic organic contaminants (HOCs) and in the subsequent evaluation of their effects on ecological and human health. HOCs freely dissolved in water ( $C_{\text{free}}$ ) will partition into the passive sampler polymer achieving an equilibrium between environmental phases (e.g., dissolved organic carbon, suspended sediments). One major challenge associated with passive sampling is ensuring that equilibrium between the polymer and the environmental phases has been attained for each HOC. Using performance reference compounds (PRCs) is one way to address this challenge. Based on the percent of PRC released during a deployment, a fractional equilibrium ( $f_{\text{eq}}$ ) or sampling rate ( $R_s$ ) can be calculated and used to extrapolate equilibrium conditions for target contaminants. Currently, there are several models used to analyze PRC data that include first order kinetic and diffusion-based processes. This study performed an in-depth analysis of PRC data using many of the common modelling methods to determine  $C_{\text{free}}$  for several polychlorinated biphenyls (PCBs). To achieve this objective, four different thicknesses of low-density polyethylene (LDPE) passive samplers were preloaded with six,  $^{13}\text{C}$ -labelled-PCBs as PRCs and deployed in the PCB contaminated New Bedford Harbor Superfund site (MA, USA). This relatively large number of PRCs and elevated target contaminant concentrations provided a robust dataset for evaluating  $f_{\text{eq}}$ ,  $R_s$ , and modeled estimates of  $C_{\text{free}}$ . Following the deployments, the percent of PRC lost ranged from 0-100% and decreased with increasing PRC size as well as

sampler thickness, allowing  $C_{\text{free}}$  comparisons for samplers at different  $f_{\text{eq}}$ . Using the different thicknesses of LDPE also allowed for further assessment of precision when using PRC models to measure  $C_{\text{free}}$  when samplers have not attained equilibrium. Overall, this investigation demonstrated the utility of PRC data for calculating  $f_{\text{eq}}$  and  $R_s$  in order to adjust target contaminants to equilibrium conditions when calculating  $C_{\text{free}}$ .