APPENDIX F. PASSIVE SAMPLER CALCULATIONS FROM THE PCB POREWATER INVESTIGATION

1 Equilibrium corrections for PCB Porewater calculations

As expected for well-agitated exposures, performance reference compound (PRC) data confirmed the polyethylene (PE) sheets were very close to full equilibrium with the sediment porewater for all samples. In six of the eleven samples, the most hydrophobic PRC (polychlorinated biphenyl [PCB] 178) was more than 90% equilibrated (Table F-1). All the PCB congeners were assumed to be fully equilibrated for these six samples.

For the other five samples, small equilibrium corrections using PRC data were required (LDW18-PWPS-174, LDW18-PWPS-174-dup, LDW18-PWPS-184, LDW18-PWPS-185, LDW18-PWPS-187). For these five samples, as specified in the quality assurance project plan (QAPP), full equilibrium was assumed for PCB congeners that had a K_{ow} lower than or equal to the most hydrophobic PRC that had a fractional equilibrium higher than 0.9 (i.e., more than 90% equilibrated) (Windward 2018). Equilibrium corrections for the remaining PCB congeners were attempted using the PRC calculator software (Gschwend et al. 2014), as described in the QAPP. However, the diffusion model used by the PRC calculator software was not always able to produce reasonable regressions for two reasons: the lack of PRC data within the required equilibrium threshold range of 10 to 90% (Gschwend et al. 2014), and the fact that all of the data were clustered close to the 90% threshold.

Two recent studies have suggested that first-order kinetics based methods should be used rather than diffusion model-based PRC corrections, like the PRC calculator software (Gschwend et al. 2014) for well-mixed systems (Apell et al. 2018; Sanders et al. 2018). Therefore, a first-order kinetics-based method described by Sanders et al. (2018) was used for the PRC corrections for the five samples identified in Table F-1. This method is based on establishing a linear correlation between the exchange rate of each PRC in each sampler and the K_{ow} of the PRC. The exchange rate can be predicted for target PCB congeners using the correlation line, then used to estimate the fractional equilibrium for each PCB congener. The correlation line for each sample was established using all PRC data < 90% equilibrated, combined with the most hydrophobic PRC that was > 90% equilibrated (Attachment F1 and Table F-1).

Table F-1. Percent equilibrium in porewater passive samplers

Sample ID	PRC -Percent Equilibrium					
	PCB-008	PCB-028	PCB-095	PCB-111	PCB-153	PCB-178
LDW18-PWPS-SS169	98.9%	98.4%	98.8%	98.2%	92.6%	94.4%
LDW18-PWPS-SS172	99.2%	100%	99.0%	98.1%	89.6%	91.3%
LDW18-PWPS-SS174	95.7%	93.5%	**94.4%**	**89.5%**	**83.3%**	**80.9%**
LDW18-PWPS-174 (DUP)	94.7%	93.1%	**94.37%**	**88.6%**	**82.4%**	**77.6%**
LDW18-PWPS-SS175	98.4%	97.3%	97.9%	97.0%	87.7%	91.9%
LDW18-PWPS-SS177	99.2%	100%	99.1%	98.3%	90.8%	91.1%

Sample ID	PRC -Percent Equilibrium					
	PCB-008	PCB-028	PCB-095	PCB-111	PCB-153	PCB-178
LDW18-PWPS-SS179	99.2%	98.5%	98.6%	97.9%	91.4%	91.4%
LDW18-PWPS-SS180	99.3%	100%	99.2%	98.7%	88.2%	90.9%
LDW18-PWPS-SS184	98.3%	97.0%	97.6%	**95.0%**	**85.2%**	**78.6%**
LDW18-PWPS-SS185	97.4%	96.3%	95.1%	**90.6%**	**79.6%**	**70.5%**
LDW18-PWPS-SS187	96.1%	94.0%	**94.5%**	**88.4%**	**78.8%**	**67.4%**

Shaded rows indicate the samples that required the first-order kinetic method to calculate the equilibrium correction, because the most hydrophobic PRCs were less than 90% equilibrated.

Bold PRC values were used to establish a linear correlation between the exchange rate of each PRC in each sampler and the K_{ow} of the PRC to estimate the fractional equilibrium for each PCB congener.

ID – identification

PCB – polychlorinated biphenyl

PRC – performance reference compound

2 References

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Windward. 2018. Lower Duwamish Waterway baseline surface sediment collection and chemical analyses - quality assurance project plan. Final. Windward Environmental LLC, Seattle, WA.