2024

# Contamination Assessment and Reduction Project – Phase 2 (CARP II)

## *Appendix A-4. Rapid Assessment of Dredged Material Quality*

# Objective 5: Evaluate methods for predicting HARS suitability:

## Develop a quick and reliable testing method for PCDD/Fs and PCBs in sediments using passive samplers for future field testing

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***Introduction***

The overall goals of the Contamination Assessment and Reduction Project II (CARP II) were to: (i) evaluate current and future contamination of New York-New Jersey (NY-NJ) Harbor sediments, and (ii) determine if and when dredged material from the harbor would meet criteria for disposal at the Historic Area Remediation Site (HARS). For current assessments, HARS suitability is based on 28-day bioaccumulation tests using the dredged material test organism *Neanthes virens* (formerly classified as *Nereis virens*). Although the 28-day bioaccumulation tests provide a justifiable method for assessing HARS suitability, bioaccumulation testing can be costly, and more importantly, test results are of limited value in evaluating HARS suitability for future projections of sediment contamination.

Therefore, the primary purpose of this task was to test whether we can design a passive sampler method in such a way that is gives a reliable indication of the sediment's contaminants potential for bioaccumulation by using a combination of (i) much thinner passive sampler material to speed up equilibration (7, 14 or 25 μm*)* and a much quicker (on the time scale of several days to a week) sampling approach to assess the bioaccumulation potential of dredged sediments. The aim was to identify a simple approach that could become a first screening tool for dredged sediments. Specific contaminants of concern in these studies were polychlorinated biphenyls (PCBs) and polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs).

Passive sampling techniques are capable of measuring the freely dissolved concentrations of hydrophobic organic contaminants (bioavailable fraction) or serving as a proxy for studying bioaccumulation in organisms[1–3]. In contrast to the traditional geochemical approaches, where pore water concentrations were predicted indirectly from sediment concentrations and organic/black carbon content[4,5], passive

samplers determine the freely dissolved concentration via diffusive uptake into the sampler matrix[3,6,7]. However, the previously published studies often suffered from large estimation errors, attributed to insufficient equilibrium partition coefficient values[1,8,9].

Therefore, we utilized the CARP II sample set, containing sediment's contaminant concentrations (PCDD/Fs and PCBs) in both pore water and in sediment dwelling biota to assess and derive new partitioning values for these contaminants. Porewater concentrations were determined by a passive sampling equilibrium experiment performed under controlled laboratory conditions, while the standard (regulatory) 28-day bioaccumulation test was relied on to derive lipid-based concentrations in sedimentary biota). The newly derived partitioning coefficients were used to improve the performance of the prediction model by reducing the relative mean standard error (RMSE) of the biota concentration values estimated from the measured pore water concentration.

The established method used to derive porewater concentrations of PCBs and PCDD/Fs relies on 7-weeks equilibration of the sediment with passive samplers in the laboratory[10]. The main constraint for the long equilibration time is the presence of an aqueous boundary layer surrounding the passive sampler and preventing quick diffusion of compounds towards the sampler. A much quicker (on the time scale of several days to a week) sampling approach would be ideal to assess the bioaccumulation potential of dredged sediments and manage the risks associated with freshly dredged material. The "quick" passive sampling results could serve as first screening approach for evaluating the HARS-suitability of dredged material and help in decision-making process. If the estimated porewater concentrations are below levels of concern, the full-blown 28-day bioaccumulation test can be performed according to the standardized U.S. EPA and USACE protocol. For dredged material that fails the quick screening test, the dredged material can be designated for disposal without additional costly and time-consuming bioaccumulation tests.

We hence proposed to perform various tests with one homogenized sediment from the Newark Bay region to determine how long we need to expose samplers to derive a robust estimation of porewater concentrations. The primary objectives of this task were therefore defined as follows:

1. Derive the most appropriate set of partitioning correlation between passive samplers and standard laboratory test animals' lipid concentrations of target contaminants.

2. Test whether a new, much thinner passive sampler material, could speed up equilibration (9, 18 or 25 µm) in sediment incubations while being able to detect compounds of concern.

3. Confirm that target compounds are in or near equilibrium from both the uptake of sediment-bound compounds, and the release of performance reference compounds over time.

4. Derive a simple model that can predict the accumulation of target compounds in the lipid of worms in standard 28-day bioaccumulation test based on the passive sampler incubations.

**Methods**

For the determination of the freely dissolved concentrations in sediment, an ex-situ equilibration experiment under controlled laboratory conditions was used based on a previously published protocol[11]. Briefly, the PE sheets were equilibrated with 250 g of sediment sample in an amber glass jars filled up with a 200 mg/L sodium azide solution (leaving sufficient headspace to allow thorough homogenization) on a laboratory shaker table (Lab Companion OS-7200, Jeio Tech, Korea) at 120 rpm for 37 days. Six blank samples were processed the same way, containing no sediment.

The LDPE sheets were cut from commercial sheeting (FilmGard, Berry Plastics Corp, USA) with a thickness of 50 µm into 2 x 3 cm strips (~160 mg). Consecutively, the sheets were precleaned with n-hexane and dichloromethane (DCM) by two 24-hour rounds and loaded with performance reference compounds (PRCs) (d8-naphthalene, d12-benzo(a)anthracene, d12-benzo(a)pyrene 2,5- dibromobiphenyl (PBB 9), 2,2',5,5'-tetrabromobiphenyl (PBB 52), 2,2',4,5',6-pentabromobiphenyl (PBB 103) and octachloronaphthalene) by equilibrating with PRC solution on a laboratory shaker table (Lab Companion OS-7200, Jeio Tech, Korea) as described elsewhere[1].

Prior to extraction, all the LDPE samples were gently wiped with laboratory-grade tissue and spiked with ISs (13C mass labelled 2,3,7,8-TCDF; 2,3,7,8-TCDD; 1,2,3,7,8-PeCDF; 2,3,4,7,8-PeCDF; 1,2,3,7,8-PeCDD; 1,2,3,4,7,8-HxCDF; 1,2,3,6,7,8-HxCDF; 2,3,4,6,7,8-HxCDF; 1,2,3,7,8,9-HxCDF; 1,2,3,4,7,8-HxCDD; 1,2,3,6,7,8-HxCDD; 1,2,3,7,8,9-HxCDD; 1,2,3,4,6,7,8-HpCDF; 1,2,3,4,7,8,9-HpCDF; 1,2,3,4,6,7,8-HpCDD; OCDD; OCDF; PCB 3; PCB 8; PCB 28; PCB 52; PCB 118; PCB 138; PCB 180; PCB 194; PCB 206; PCB 209). LDPEs were cold extracted in two rounds, 24 hours each with n-hexane and dichloromethane. The extract was concentrated under gentle stream of nitrogen and transferred into a 1 mL GC conic vial, solvent exchanged to nonane and finally concentrated to ~50 µL. 2,4,6- tribromobiphenyl and 13C 1,2,3,4-TCDD were added to all samples as recovery standards. A 10uL aliquot of the sample was sent to an accredited lab (SGS AXYS) for analysis of PCDD/Fs according to USEPA 1613 method. For the analysis of PCBs, 1 uL of the sample was injected to Agilent 6890A GC equipped with a 60 m x 0.25 mm x 0.25 µm DB5-MS UI column (Agilent J&W, USA) and coupled to a Quattro Micro (Waters, Micromass, UK) tandem mass spectrometer (MS/MS). The mass spectrometer was operated in positive electron ionization impact mode (EI+) using multiple reaction monitoring (MRM). At least two transitions were recorded for each congener. Injection was splitless 1 µL at 280°C, with He as the carrier gas at 1.2 mL·min$^{-1}$. The GC temperature program was 120°C with a 2 min hold, then 20°C·min$^{-1}$ to 180°C, followed by 2°C·min$^{-1}$ to 260°C with a 4 min hold and 5°C·min$^{-1}$ to 315°C.

The lipid-water partitioning coefficients were calculated as:

$$K_{Lip-W} = \frac{C_{lip}}{C_{PW}} \quad \text{(Eq 1)}$$

Where the concentration in pore water ($C_{PW}$) was calculated from concentration in LDPE passive samplers and PE-water partitioning coefficient $K_{PE-W}$ according to[8] and concentration in lipid was measured.

Literature $K_{lip-W}$ values were calculated from $K_{OW}$ using following previously published equation[12]:

$$\log K_{LIP-W} = 1.01 \log K_{OW} + 0.12 \quad \text{(Eq 2)}$$

$K_{OW}$s were taken from[13,14].

For rapid sampler evaluation, we performed various tests with a homogenized composite sediment sample and test the approaches listed above to determine the sufficient length of the passive sampler's exposure to derive a robust estimation of porewater concentrations.

To reach this goal, three different thicknesses (9, 18 and 25 µm) of LDPE sheets (in triplicate) were equilibrated with homogenized sediment from the Hackensack river in order to determine the freely dissolved concentrations of the targeted compounds in the sediment the same way as described above. Triplicates of each sheet thickness were equilibrated for 2, 4, 8, 12 and 16 days.

The LDPE sheets for this experiment were prepared as follows: approximately 0.5g strips were cut from commercial sheeting (FilmGard, Berry Plastics Corp, USA) and consecutively precleaned with n-hexane and dichloromethane (DCM) by two 24-hour rounds and loaded with performance reference compounds (PRCs) (PCB 2, 14, 30, 50, 104 and 145) by equilibrating with PRC solution on a laboratory shaker table (Lab Companion OS-7200, Jeio Tech, Korea) as described elsewhere[1].

After the equilibration experiment was finished, all the collected PE sheets were extracted and analyzed for the content of PCBs and PRCs as described above. The sample was injected to Agilent 7890A GC equipped with a 30 m x 0.25 mm x 0.25 µm DB5-MS UI column (Agilent J&W, USA) and coupled to an Agilent 5977 mass spectrometer (MS). The mass spectrometer was operated in positive electron ionization impact mode (EI+) using single ion monitoring (SIM). At least two masses were recorded for each congener. Injection was splitless 1 µL at 280°C, with He as the carrier gas at 1.2 $mL \cdot min^{-1}$. The GC temperature program was 120°C with a 2 min hold, then 20°C·$min^{-1}$ to 180°C, followed by 2°C·$min^{-1}$ to 260°C with a 4 min hold and 5°C·$min^{-1}$ to 315°C.

Commercially available standards of the 29 targeted PCB congeners (PCB 8, 11, 18, 28, 52, 44, 66, 81, 77, 101, 123, 118, 114, 105, 126, 153, 138, 128, 167, 156, 157, 169, 187, 180, 170, 189, 195, 206, 209) and six performance reference compounds (PCB 2, 14, 30, 50, 104 and 145) (Accustandards) were used to construct a seven point calibration curve in order to determine the concentration of the analytes in the samples.

EPA's regulatory cutoff for sediment concentration is based on a human health endpoint, calculated form the reference dose listed in the EPA IRIS database for non-cancer effects, and has been calculated as 113 ppb total PCBs on a wet weight basis in the benthic animals (taking into account food-chain enrichment). A factor of 2 is used by US EPA to extrapolate from the targeted 22 PCB congeners to total PCBs, which was validated as appropriate for estimating total PCB mass using various NY/NJ Harbor datasets that reported extended congener lists in various environmental media. For our purposes, the 113 ppb threshold values was converted to a lipid based concentrations using the mean lipid content of 1.6% from the experimental results. This resulted in a target concentration of 6,900 ng total PCBs per g lipid. Lipid-based concentrations were calculated from PCB concentrations measured in passive samplers as:

$$C_{lip} = \frac{C_{PE} \cdot K_{LIP-W}}{K_{PE-W}} \quad \text{(Eq 3)}$$

where

$c_{PE}$ represents the average of the triplicate measurement of the PCB concentration in the passive sampler (ng/g)

$K_{LIP\text{-}W}$ is the lipid-water partitioning coefficient

$K_{PE\text{-}W}$ is the sampler-water partitioning coefficient

No equilibrium correction was applied.

Our analytical method included 29 PCB congeners, though not all the same as the one EPA targeted. For the reasons outlined above, we included a factor of 2 to extrapolate to total PCBs.

## Results and Discussion

1. *Derive the most appropriate set of partitioning correlation between passive samplers and standard laboratory test animals' lipid concentrations of target contaminants.*

As described in detail in the method section above, we used our unique sample set derived during CARP II (task 5) of measured $C_{PW}$ and $C_{lip}$ to calculate $K_{LIP\text{-}W}$ values from Eq 1 and derive new $K_{LIP\text{-}W}$ vs $K_{OW}$ relations (Fig.1 and 2). These measurements are representative of a wide range of sediments present in the New York-New Jersey Harbor region, and thus represent the most suitable set of partitioning relationships for the prediction of bioaccumulation of target contaminants for CARP II.

Different behavior of PCDDs, PCDFs and PCBs was observed and therefore three different sets of $K_{LIP\text{-}W}$ were derived for each compound group (Table 1). The newly derived $K_{LIP\text{-}W}$ calculations were then used to calculate $C_{lip}$ estimations and their prediction errors to demonstrate the capability of the LDPE sampler to successfully predict the concentrations of the pollutants in biota (Fig. 3) as well as for comparison of measured concentrations to US EPA regulatory cutoff criterium.

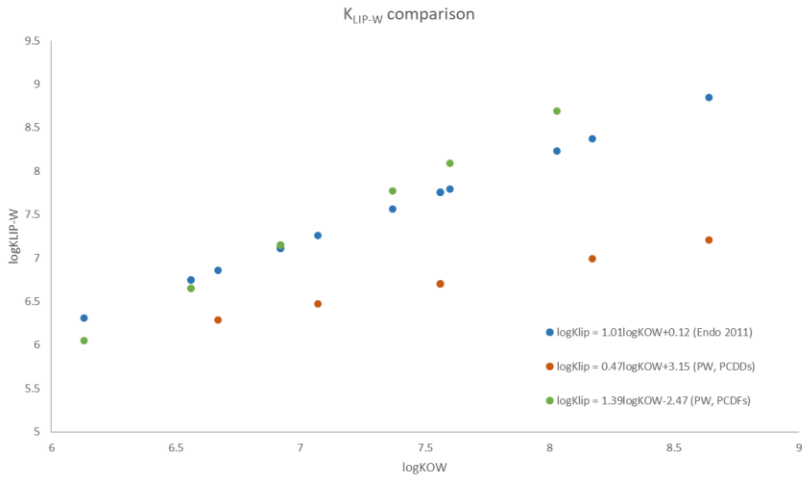

**Fig.1 Comparison of literature $K_{LIP-W}$ relation on $K_{OW}$ for PCDD/Fs and newly derived relation based on pore water and lipid measurements.**

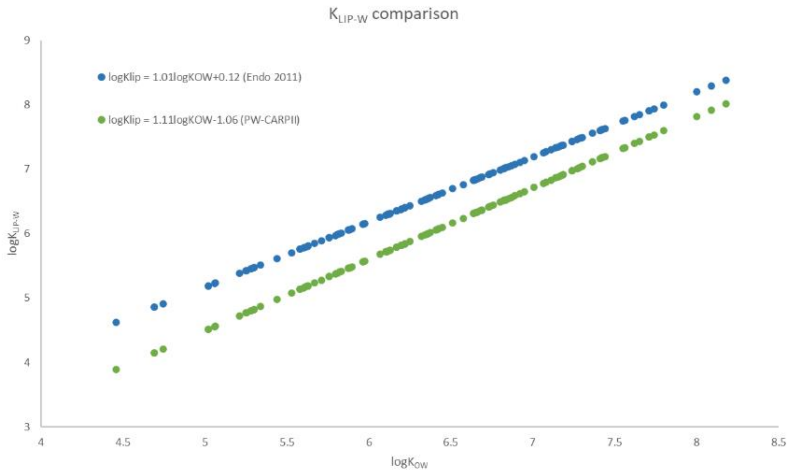


**Fig.2 Comparison of literature $K_{LIP-W}$ relation on $K_{OW}$ for PCBs and newly derived relation based on pore water and lipid measurements.**

Table 1 summarizes the results from task 5, and the set of equations to be used in this task. Note that the relationships derived here differ from generic literature values; however, the equations for PCBs, PCDDs and PCDFs are specific to the New Jersey-New York harbor region and thus preferable.

**Table 1: Comparison of newly derived $K_{LIP-W}$ and $K_{OW}$ relations.**

| | Equation |
|---|---|
| Literature (PCDD/Fs, PCBs)[12] | $\log K_{LIP-W} = 1.01 \log K_{OW} + 0.12$ |
| PCDDs | $\log K_{LIP-W} = 0.47 \log K_{OW} + 3.15$ |
| PCDFs | $\log K_{LIP-W} = 1.39 \log K_{OW} - 2.47$ |
| PCBs | $\log K_{LIP-W} = 1.11 \log K_{OW} – 1.06$ |

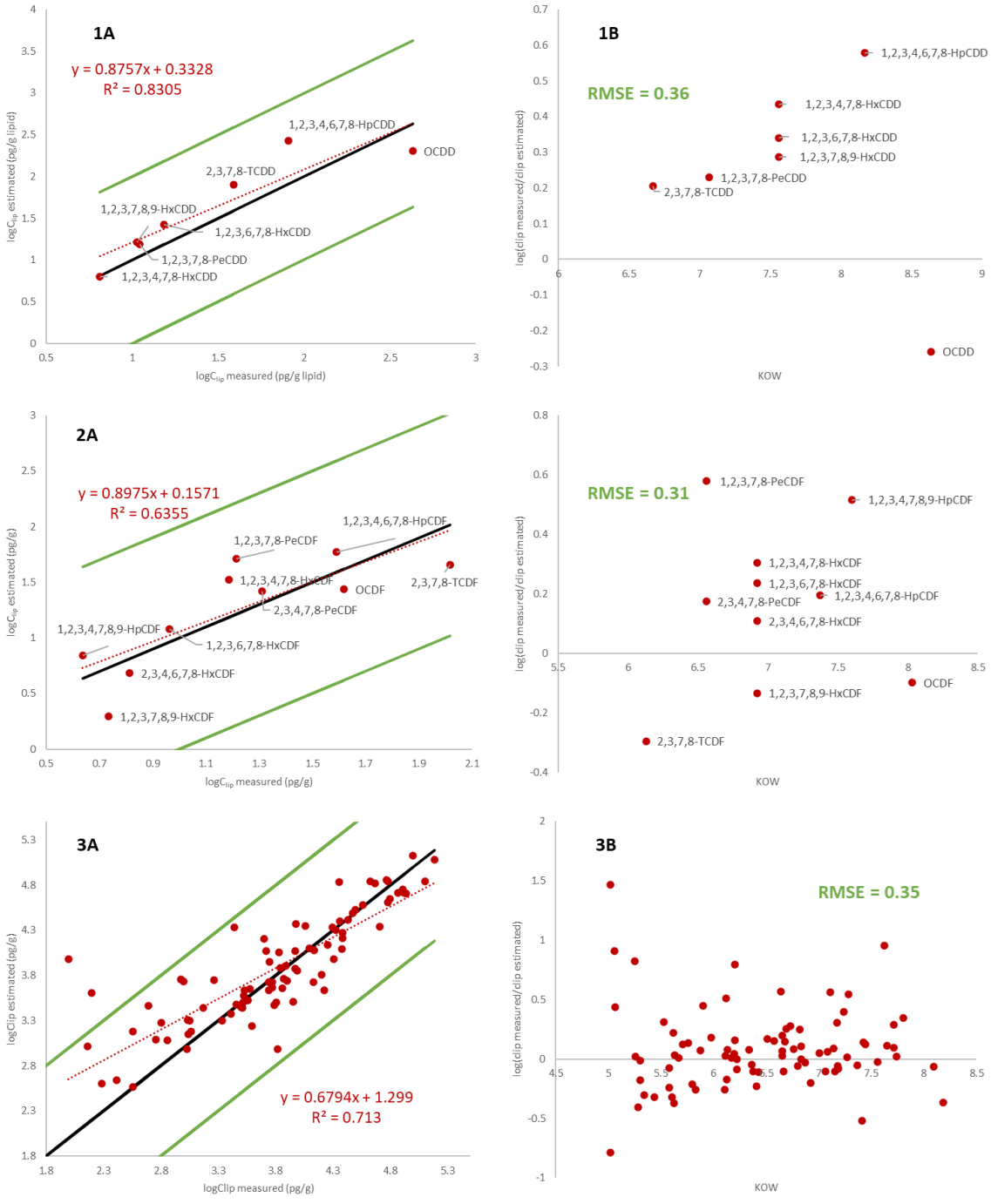


**Fig 3. Comparison of lipid concentrations (A) and the predicted/measured values ratio versus log$K_{OW}$ (B) of PCDDs (1), PCDFs (2) and PCBs (3) predicted from the concentrations in LDPE samplers using the pore water model versus concentrations directly measured in the biota lipid. Points represent average values across the samples. The solid black line represents Cest = Cmeasured, green line represents plus and minus factor of ten, red dotted line represents best fit of the data.**

2. *Test whether a new, much thinner passive sampler material, could speed up equilibration (9, 18 or 25 µm) in sediment incubations while being able to detect compounds of concern.*

Eight native PCB congeners were detected in the passive samplers at concentrations ranging from 33 ng/g of PE to 418 ng/g of PE per congener. In general, no significant differences in the concentration were observed at the equilibrium between the sampler thicknesses. Concentrations normalized per mass of the passive samplers showed very similar concentrations for PE sheets of either 9 μm (blue), 14 μm (grey) or 25 μm (orange) (Fig. 4). Up to hexa-chlorinated PCB congeners (PCB 28, 52, 81, 118, 153, 105 and 138), the equilibrium was reached by day four of the exposure for all sampler thicknesses (Fig.4).

Some differences in the uptake rate were observed for hepta-chlorinated PCB 180, where the 18 and 25 um samplers reached the equilibrium after 16 days from deployment, while the thinnest 9 um sampler reached the equilibrium much faster, at day 8, which would be extremely beneficial for the rapid screening purposes. Overall, though, 4 days seems sufficient, as the majority of PCBs, and PCB mass, already accumulated after 4 days in the PE sheets of different thickness. In the thinnest, 9 um, PE sheets, most PCB congeners already reached equilibrium after 2 days. This shows that a much faster equilibration time can be achieved, is feasible, and provides robust results for screening purposes.

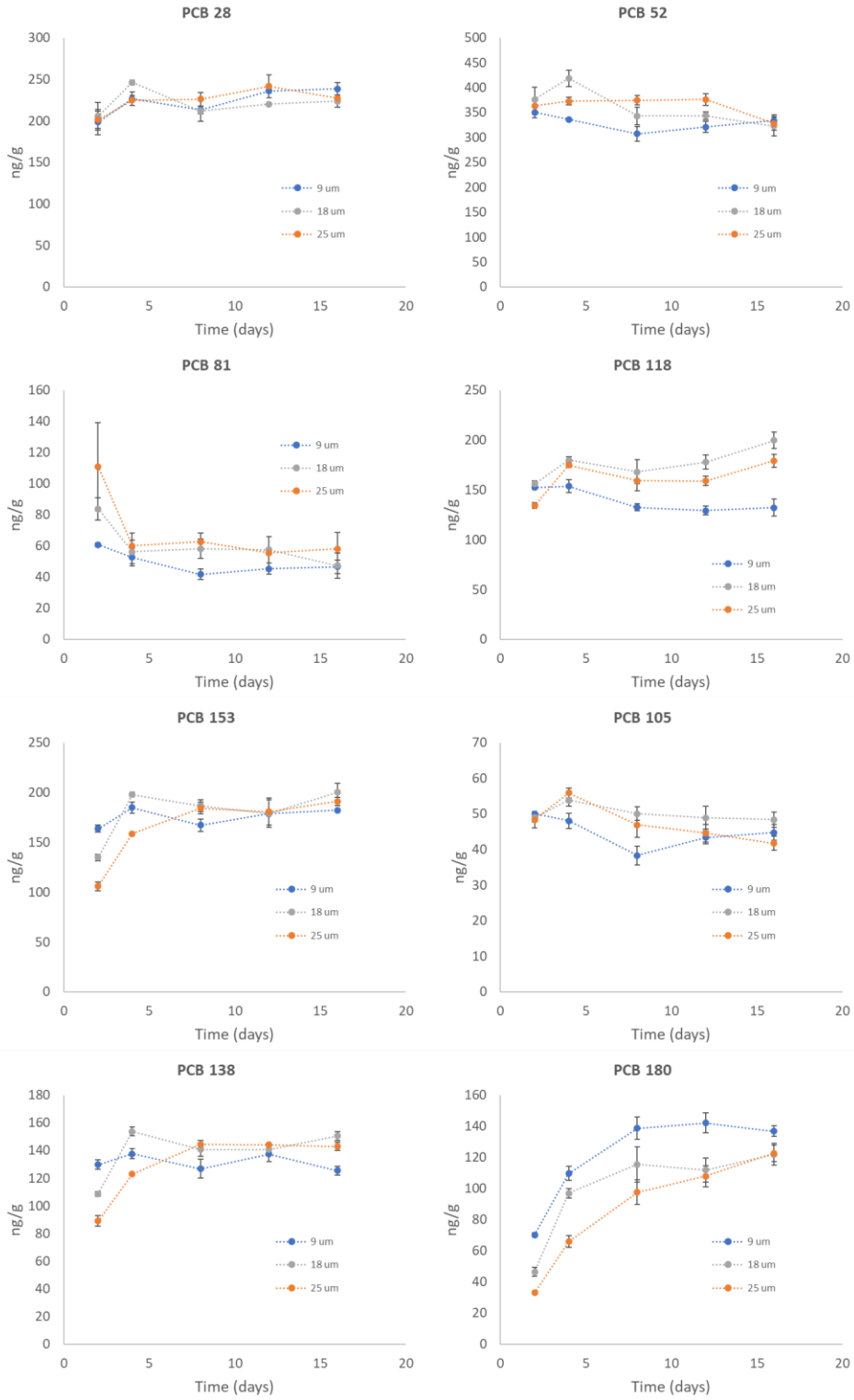


**Fig.4: The uptake curves of the detected target tri- (PCB 28), tetra- (PCB 52, 81), penta- (PCB 118, 105), hexa- (PCB 153, 138) and hepta-chlorinated (PCB 180) PCB congeners for three different sampler thicknesses.**

3. *Confirm that target compounds are in or near equilibrium from both the uptake of sediment-bound compounds, and the release of performance reference compounds over time.*

A similar pattern was observed monitoring the release of pre-loaded PRCs (consisting of PCBs with various chlorination degree) from the PE samplers (Fig. 5). The PRC release data showed that > 90% equilibration is achieved within 2 days of deployments for all congeners up to six chlorines, in support of the uptake observed (Figure 5). As is shown below, congeners 2, 14, 30 and 50 are lost rapidly within 2 days, typically decreasing to < 10% of their original values. Note that PRCs are not decreasing to zero as these experiments were performed in small batch experiments, where the PCBs reach equilibrium among sediment, water and passive sampler.

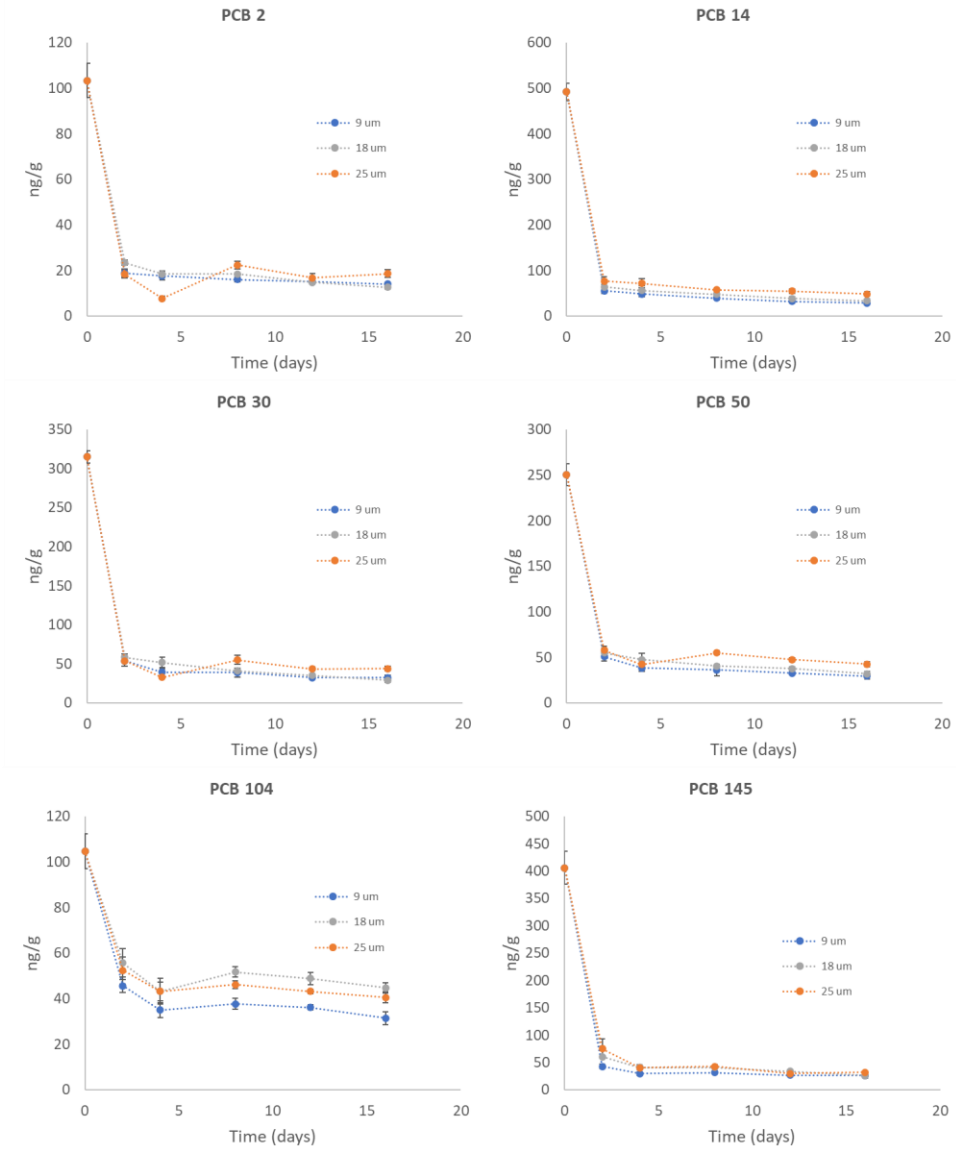

**Fig. 5: PRC release curves of six PCB congeners for three different sampler thicknesses. The chlorination level of the used PCB congeners increased by one atom of chlorine from mono- (PCB 2) to hexa- (PCB 145) chlorinated.**

The agreement between the time-scale of contaminant uptake and loss of performance reference compounds can be demonstrated by plotting a selected PRC (PCB 145) against a corresponding (same chlorination level) target PCB (PCB 153), where the uptake curve of the native PCB mirrors the release curve of the PRC (Fig.6). This is in support of the observation that equilibrium within these passive samplers membranes happens very quickly, and that PRCs can be used to verify the degree of equilibrium achieved.

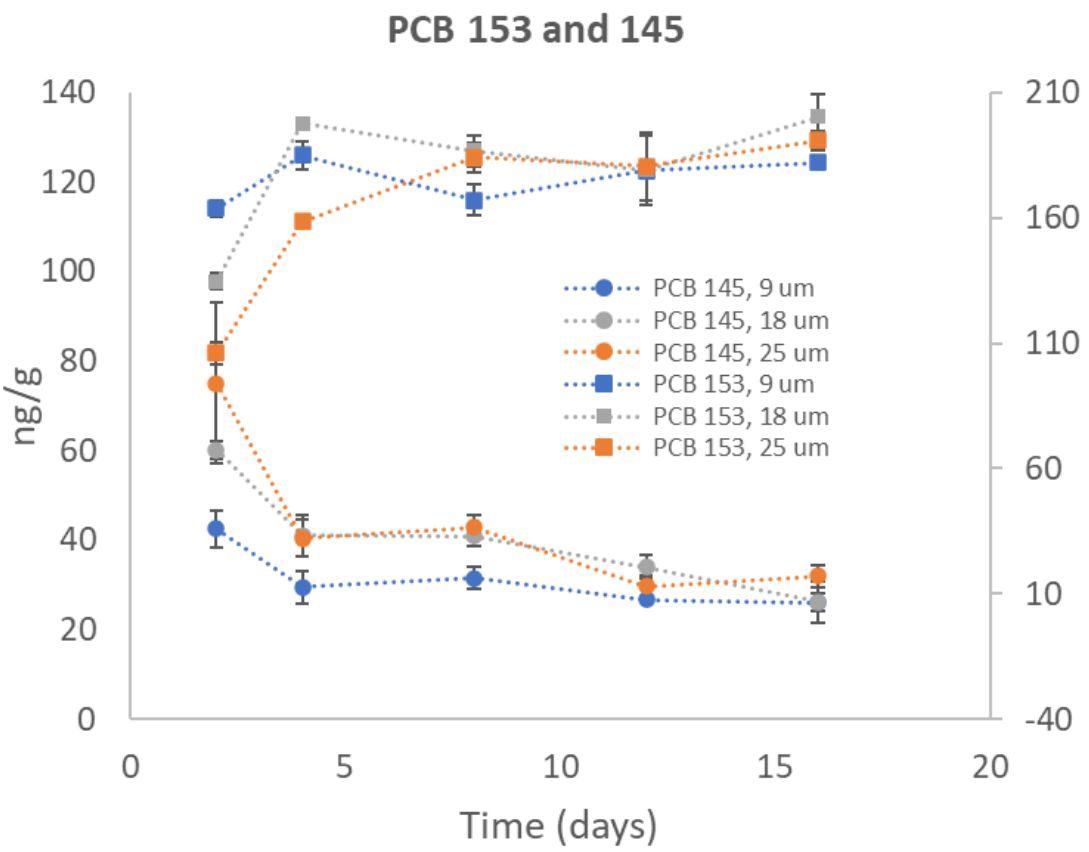


**Fig.6: Uptake (PCB 153) and release (PCB 145) curves of two hexachlorinated PCBs. PCB 153 is a target analyte, while PCB 145 was added to the passive sampler, and served as a performance reference compound.**

4. *Derive a simple model that can predict the accumulation of target compounds in the lipid of worms in standard 28-day bioaccumulation test based on the passive sampler incubations.*

When comparing our experimental data to the EPA's regulatory cutoff (Fig.7), we were able to demonstrate that LDPE-sheet based passive sampler design is sufficient to serve as a rapid and reliable tool for screening of the bioaccumulation potential of the dredged sediments. Even after only four days of deployment, the bioaccumulation potential of the PCBs in the sediment can be assessed by comparing it to the regulatory cutoff, without the necessity of costly sediment analysis. However, in order to make sure that the higher chlorinated PCB congeners reach the equilibrium, it would be preferable using the 9 um LDPE sheet sampler to be deployed for eight days. If a quick turnaround is preferred, 4 day deployments are likely sufficient and will represent a good compromise between most congeners reaching equilibrium, while minimizing deployment times. If wanted, some additional uncertainty factor can be used to account for the possibility that some of the congeners with 6 or more chlorines will not have reached equilibrium. However, at least in the case of the Hackensack River sediment, the higher chlorinated PCB congeners do not add much mass to total PCBs (Figure 7).

The concentrations of the congeners per g of LDPE sheets can then be compared to the US EPA regulatory cutoff criterium, following equation (3). The US EPA cutoff criterium is based on total PCB reference dose for non-cancer effects, converted to wet fish tissue (muscle) concentration of 113 ppb. The total PCBs are calculated as sum of 22 individual congeners, multiplied by a factor of 2, which was validated as appropriate for estimating total PCB mass.  for all LDPE sheets and all deployment lengths, total PCBs are above the regulatory cut-off, and there is no observed benefit to deploying the LDPE sheets beyond 4 days.  In this hypothetical example, we would suggest not undertaking the time and expense of the full

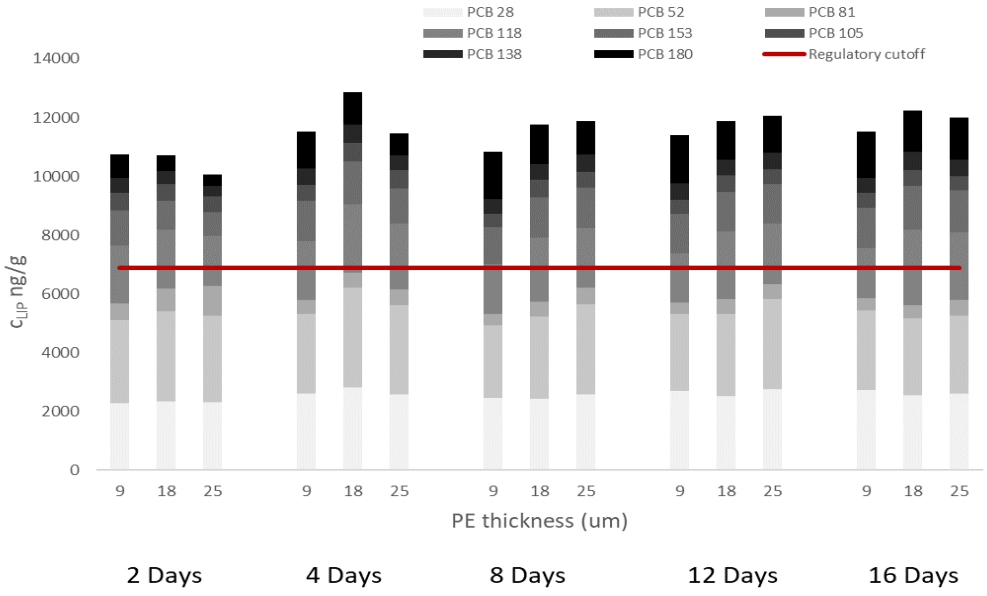


**Fig. 7: Comparison of sum of measured PCBs converted to concentrations per gram of lipid (bar graphs) with the EPA's regulatory cutoff (red line). Measured concentrations were adjusted by a factor of two to account for missing PCB congeners.**

28-day bioaccumulation test under the assumption that the sediment would be unlikely to pass the HARS criteria for ocean placement.

As demonstrated previously in the task 5, the concentration in the lipids can be successfully estimated from the concentration in the LDPE sampler (Fig 3) for PCBs and PCDFs, where over 60% of the total variance can be explained by passive sampler-derived porewater concentrations. For PCDDs, the predictive ability is less strong, which can partially be explained by poor detection frequency of the PCDDs in the passive samplers.

***Conclusions***

Passive sampling technique was successfully demonstrated to be a quick and reliable screening tool for indication of the bioaccumulation potential of legacy contaminants in dredged sediments. The unique set of empirical data, collected under the CARP II was utilized to derive the most appropriate set of partitioning correlations between passive samplers and sediment biota lipid concentrations of target contaminants. These newly derived relations were consecutively used to demonstrate the capability of the LDPE sampler to successfully predict the concentrations of the pollutants in biota.

The desired quickness of such screening process was tested in a time-sensitive laboratory equilibration experiment, which showed, that after only two days, the majority of PCB congeners already reached equilibrium. Thus, for screening purposes a laboratory incubation period of the sediment with a polyethylene passive sampler of 18 or 25 μm thickness for 2-4 days is sufficient. The obtained LDPE concentration can then be compared with the US EPA regulatory cutoff criterium in order to help in decision-making process for HARS-disposal suitability of dredged material.

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