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Polyethylene Devices (PEDs):

Customizable Tools for Unique Applications in a Variety of Environmental Scenarios

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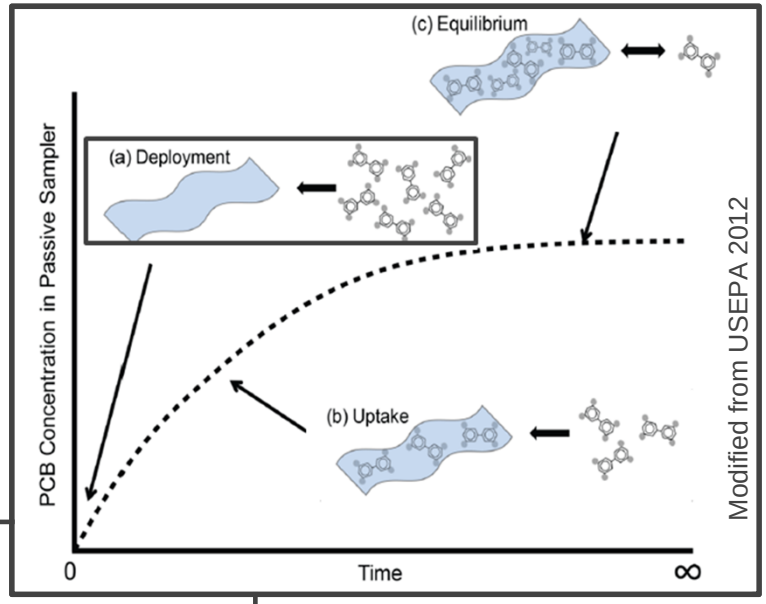
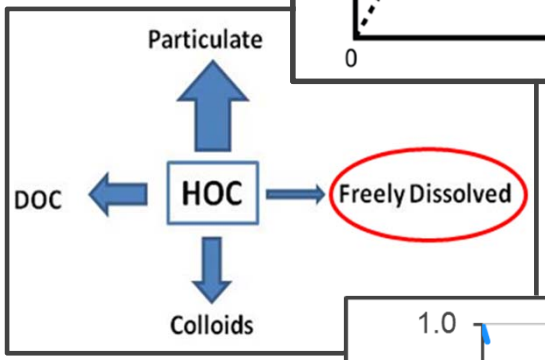
How it works

- **At equilibrium**, dissolved water concentration (C_d):

$$C_d = \frac{C_{PED}}{K_{PED}} \quad , \quad K_{PED} \propto K_{OW}$$

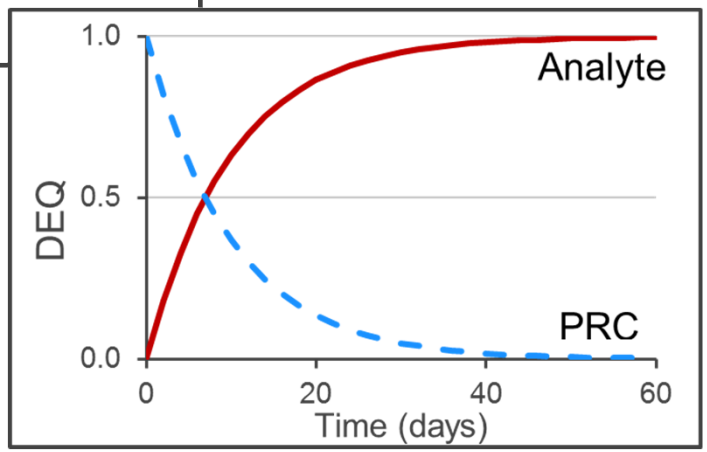




- **During uptake phase**

$$C_d = \frac{C_{PED}}{K_{PED} \cdot DEQ}$$

where *DEQ* = degree of equilibration, determined from the loss of PRCs



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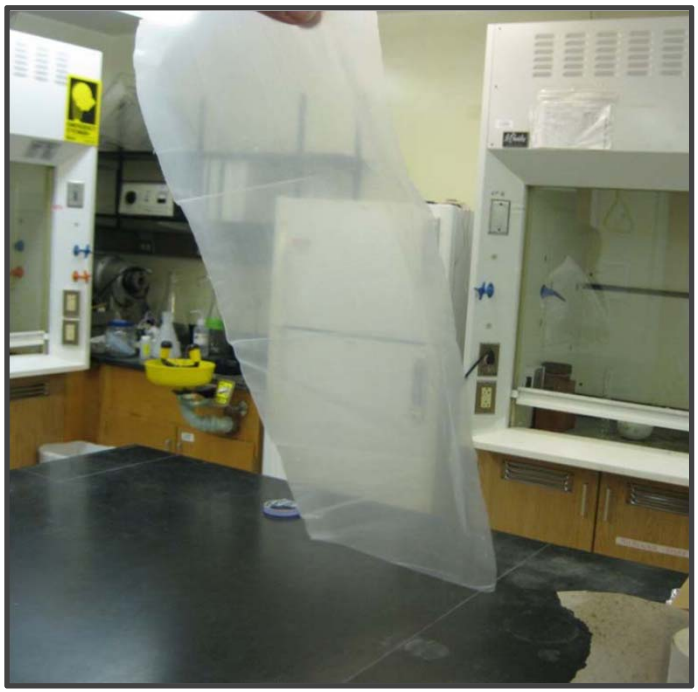
Case Study:

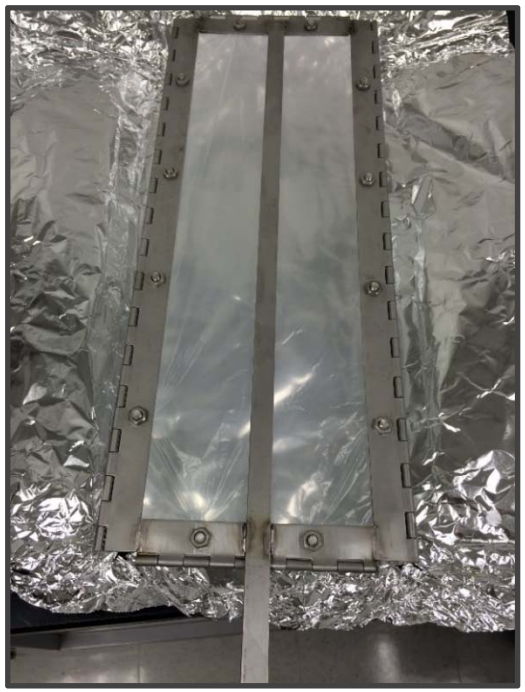
PCB-contaminated estuarine harbor

- **Site:**
  - estuarine harbor contaminated with high levels of PCBs
  - tidally influenced; salinity ~30 ‰; water depth 4 -10 feet
- **Project goal:**
  - Aid remedy design
  - Collect porewater and surface water PCB data and calculate diffusive PCB flux
- **Research goal:**
  - Conduct in situ vs. ex situ passive sampling comparison
  - Investigate reproducibility of the in situ and ex situ results

Methods - PEDs preparation

- Made from 25 µm-thick low-density polyethylene sheets
- Cut to 40 x 14 cm size and cleaned
- Spiked with performance reference compounds (PRCs); 2 PEDs per batch retained at the lab to determine PRC concentration at $t = 0$
- Framed, then wrapped for transport to the site





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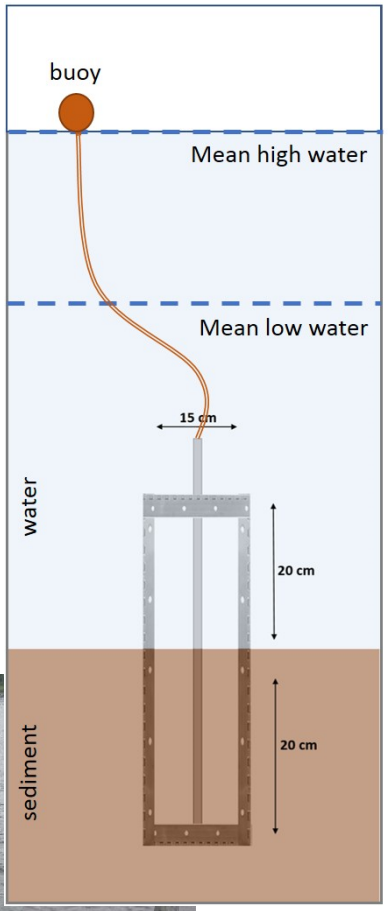
Methods - deployment

In situ PEDs:

- PEDs deployed at 22 sites (plus 3 field duplicates)
- Deployment time: 34 days

Ex situ PEDs:

- Sediment grabs collected from 18 co-located stations
- Size of PED selected to provide minimal depletion
- Lab exposures conducted by sediment slurry method in jars agitated on an orbital shaker



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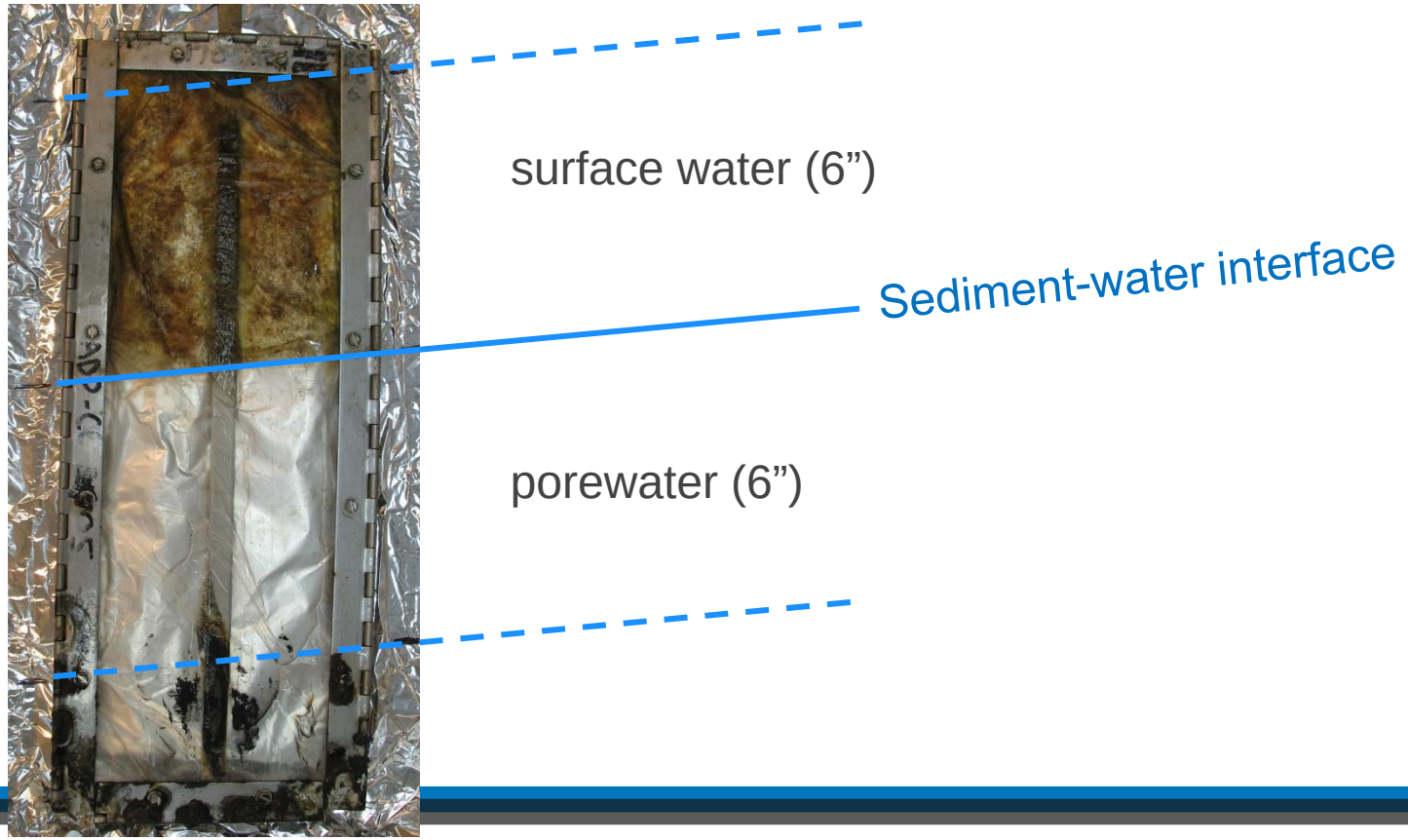
Methods – retrieval and sample prep

- PEDs from field deployments: retrieved, rinsed, photographed, shipped to the lab. At the lab: photographed, cleaned, subsectioned, extracted.
- PEDs from lab exposures: retrieved, cleaned, extracted.



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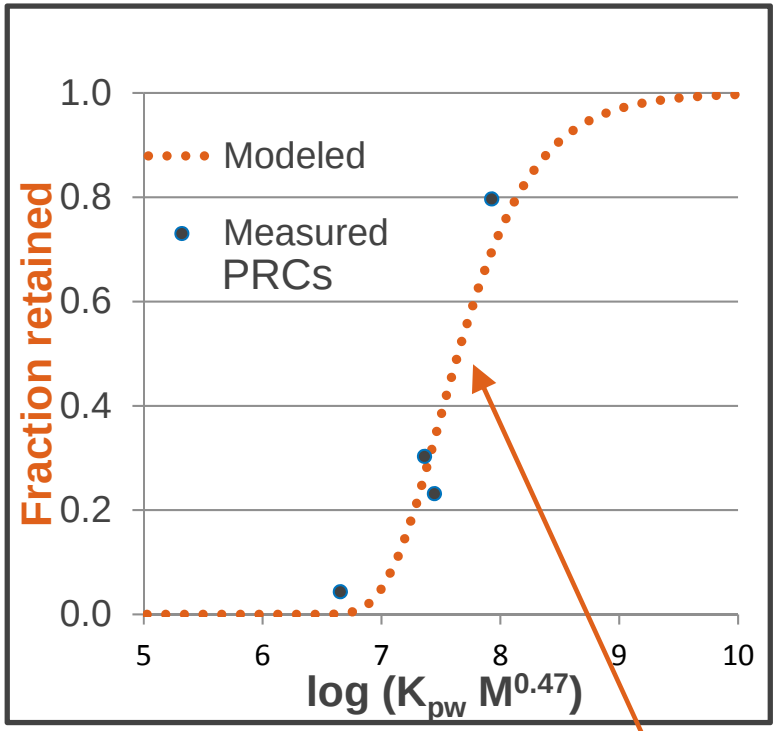
Methods – data analysis

- PED extracts analyzed in Battelle's Norwell, MA lab for 139 PCBs using modified EPA method 8270D
- Lab results (C_{PED}) reported in ng/g-PED
- **Sampling rate** (**Rs**) model used to determine DEQ for each congener based on the loss of PRCs:

$$DEQ = 1 - f_{MODELED}$$

- Dissolved water concentration (C_d) calculated for each congener as:

$$C_d = \frac{C_{PED}}{K_{PED}\ DEQ}$$



$$f_{MODELED} = \exp\left(-\frac{FAM^{-0.47}\ t}{m_p\ K_{pw}}\right)$$

FA – fitted parameter
M – molecular weight
t – exposure time
m_p – weight of PED
K_{pw} – PED-water partition coefficient

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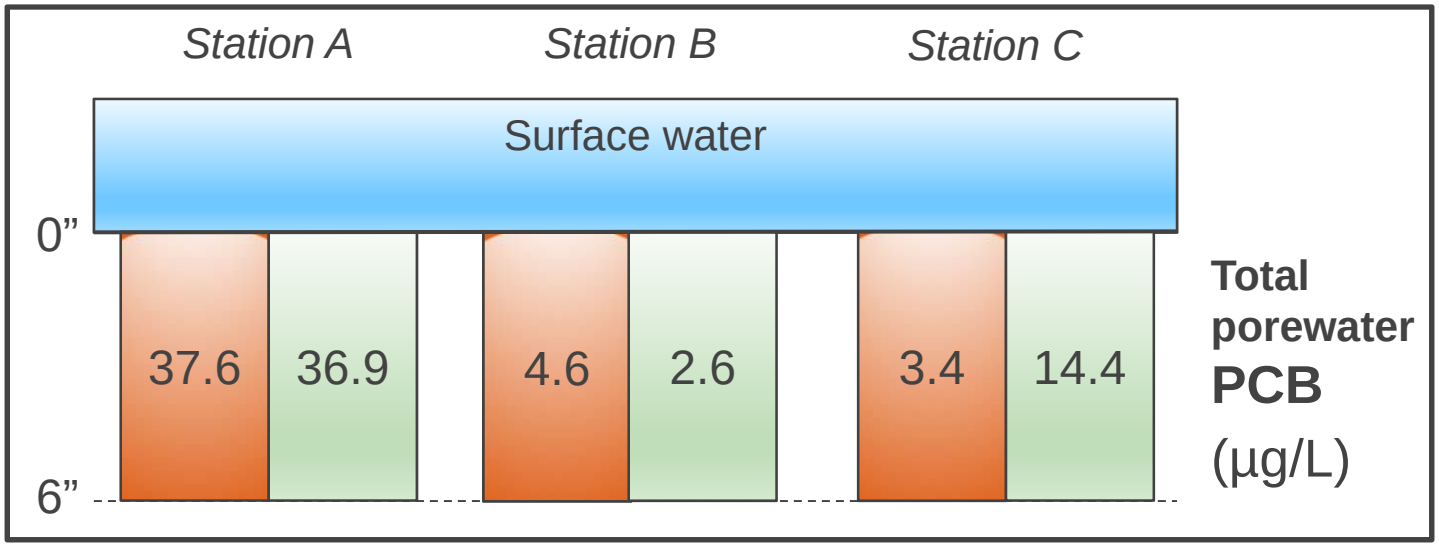
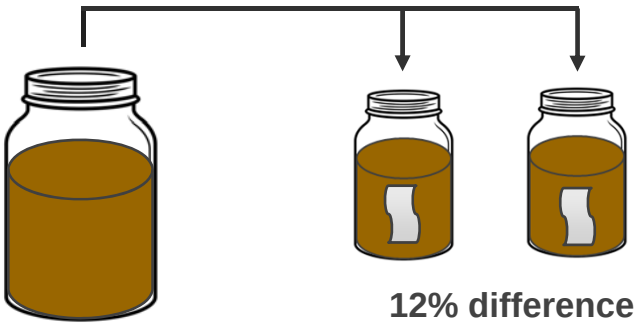
Results – measurement variability

- Equilibrium achieved for all lab exposures but not for field exposures
- Field dups (in situ):



- Lab reps (ex situ):



12% difference (average from 3 sets of duplicates)

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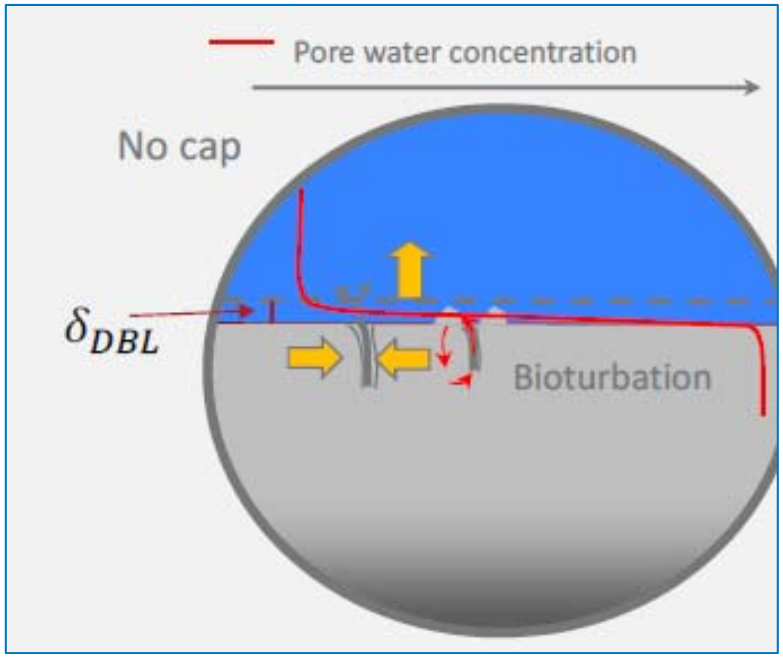
Results – diffusive flux

concentration gradient

$$F = -D_W \frac{(C_W - C_{PW})}{\delta_{BL}}$$



Eek and Reible, 2016

Where:

F	contaminant flux (positive when flux is from sediment to the water column)
D_W	diffusivity of total PCB in water
δ_{BL}	boundary layer thickness (0.02 cm; Fernandez et al. (2014)),
C_W	PCB concentration in the water column (calculated from PED data)
C_{PW}	PCB concentration in the porewater (calculated from PED data)

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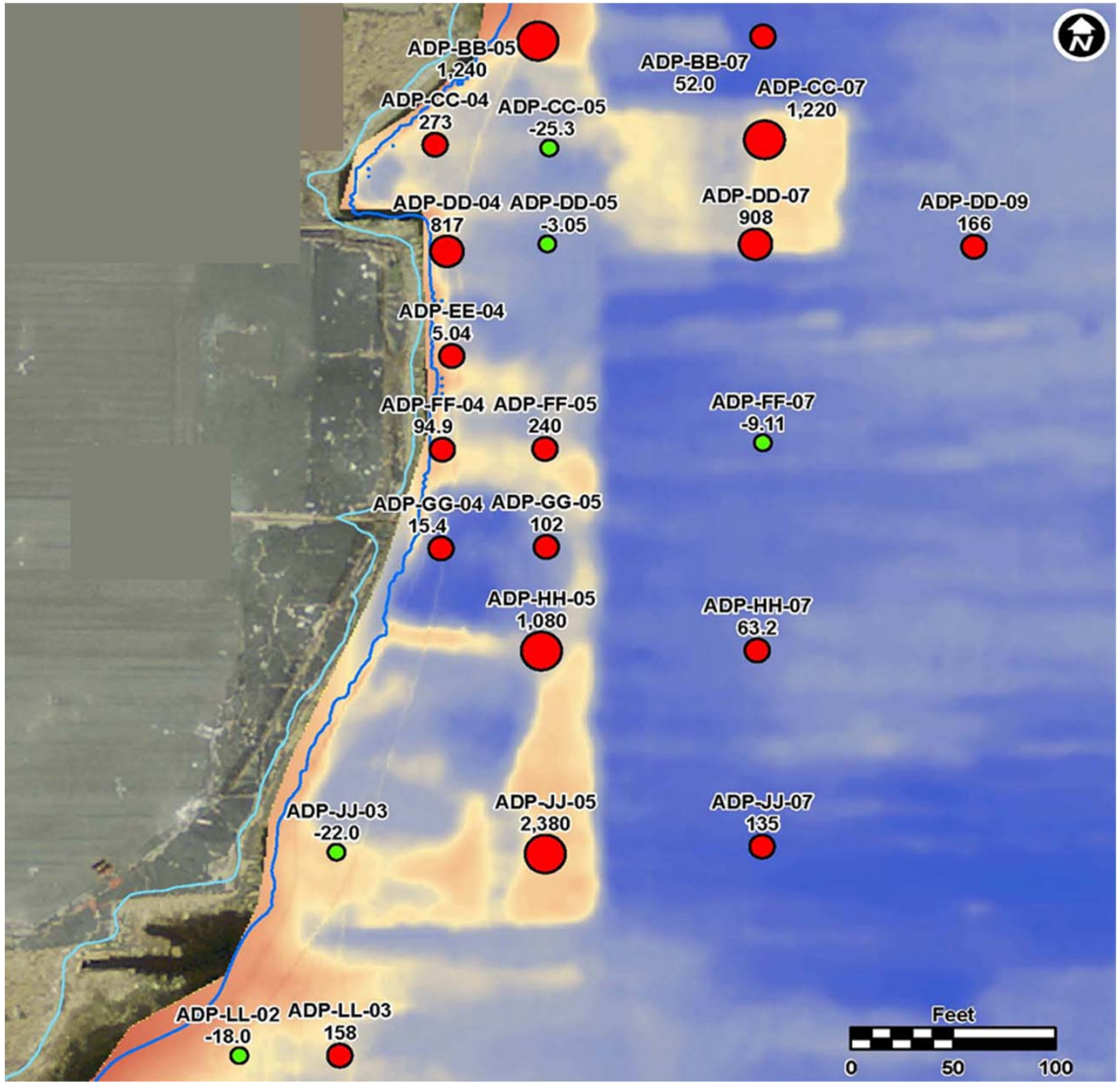
Results – diffusive flux



Flux of PCBs

(mg/m^2/yr)

- **Positive**; from sediment to surface water
- **Negative**; from surface water to sediment

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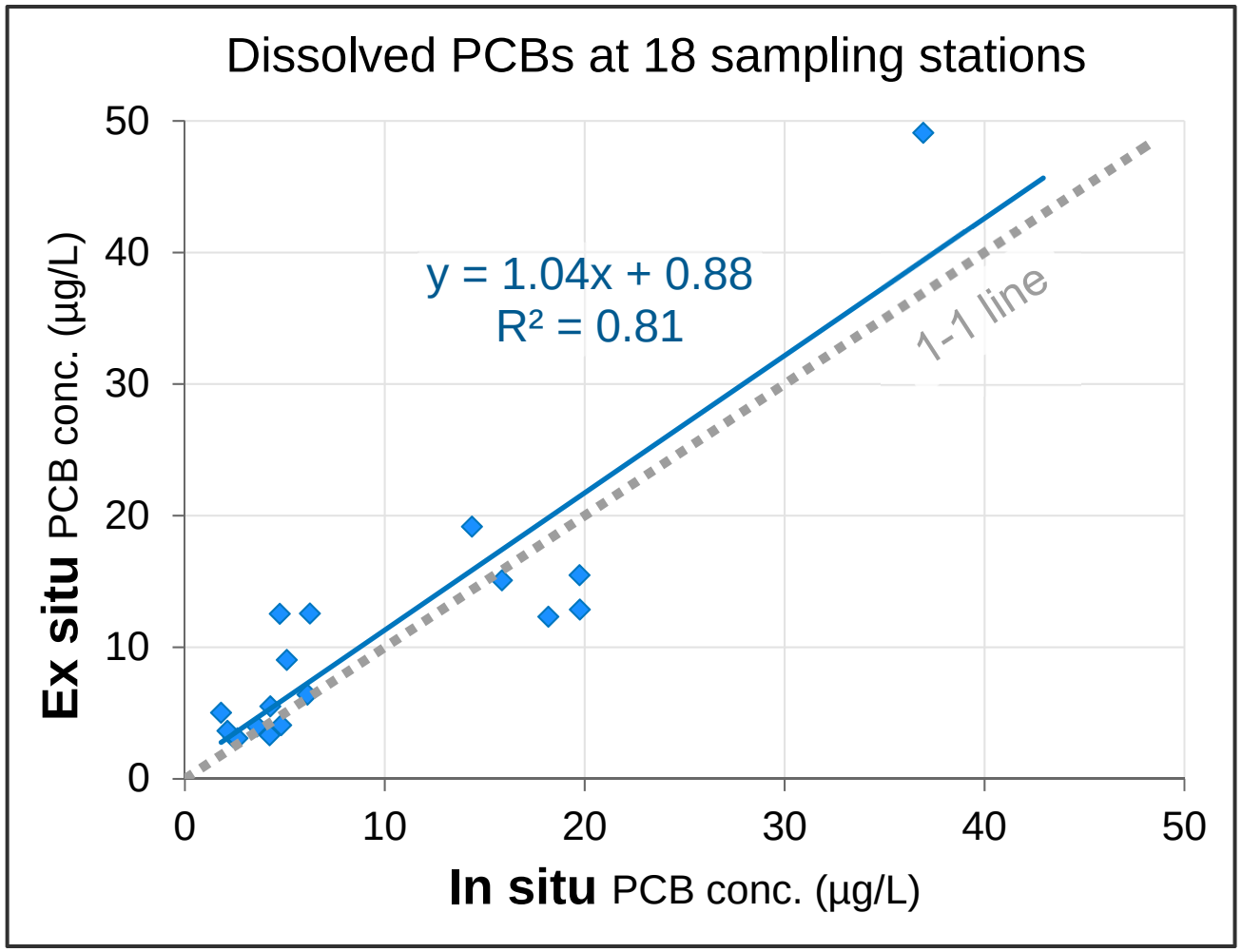
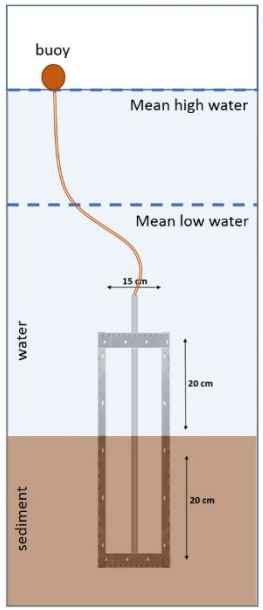
Results – in situ vs ex situ





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Case Study – Summary

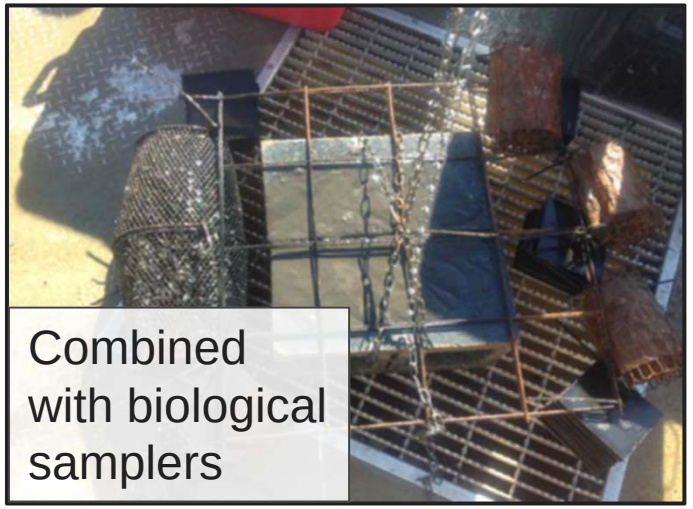
- PEDs used in **remedy design** to provide information on the concentration and flux of freely dissolved hydrophobic contaminants.
- **Ex situ** (lab) offer **comparable** results to in situ exposures and can be used when in situ deployments are difficult or risky due to significant water depths or high boat traffic.
- Ex situ exposures allow more cost-effective determination of site average contaminant concentration through compositing of sediment grab samples.

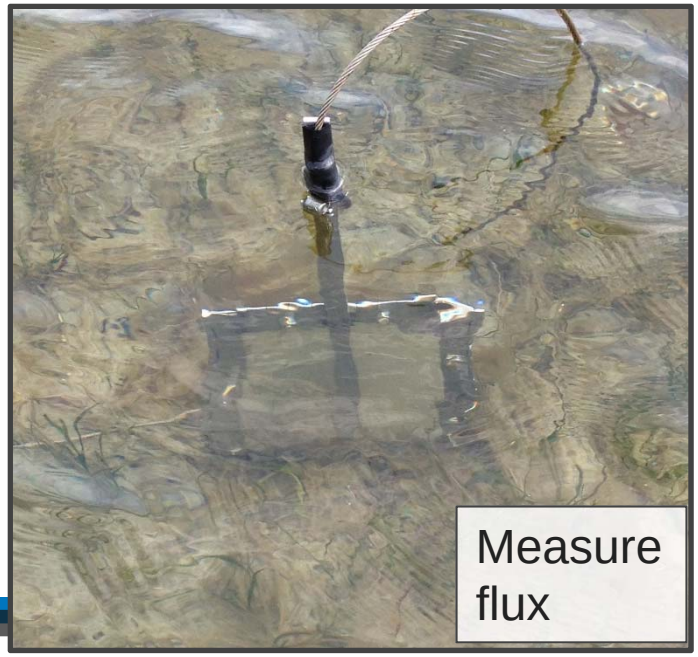
Other applications

- Improved DLs allow forensics/fingerprinting
- Combined for site investigation


In piezometers for deep porewater or groundwater measurements


In groundwater monitoring wells


Combined with biological samplers


Measure flux

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Summary – Application of PEDs

Benefits

- Measures only freely dissolved (most bioavailable) contaminants
- Easily adjustable shape and size; robust
- Better detection limits than water sampling; inexpensive
- Time-averaged results

Assumptions

- Known partition coefficients
- PRCs present analogous properties to analytes and allow determination of fractional equilibration

Applications

- Measurement of hydrophobic contaminants in surface water, groundwater, porewater
- Diffusive flux calculation for remedy design and/or monitoring
- Source tracking and forensics

Mass transfer models

- First order – simplest, for surface water.
- Diffusion – for porewater only (surface water coming soon); 0.1>PRC DEQ>0.9
- **Sampling rate (Rs)** – used in this study; suitable for porewater and surface water

QUESTIONS?

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It can be done