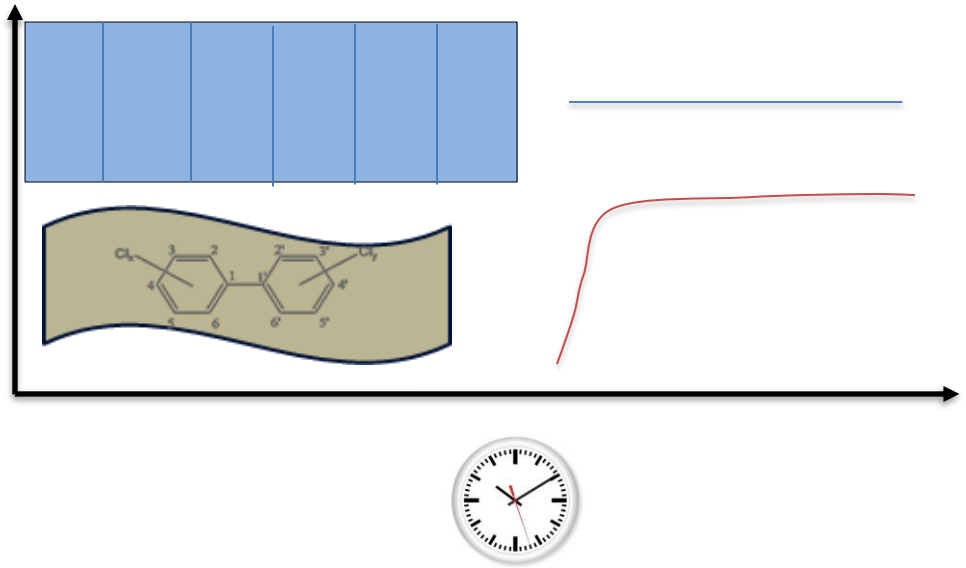
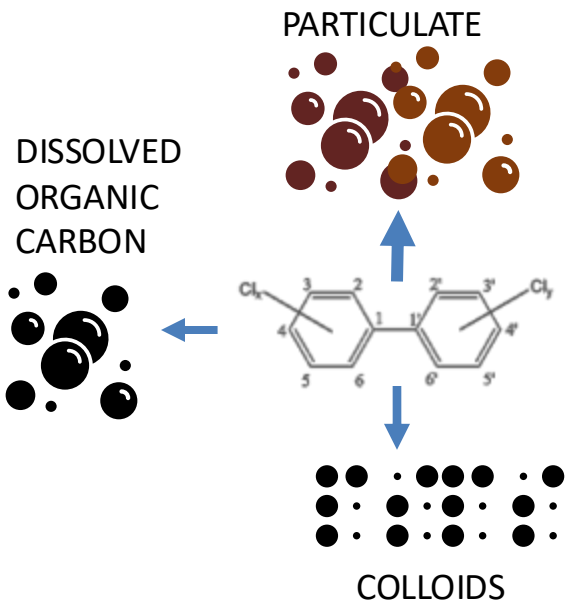
How Efficient is Time-Integration for Equilibrium Passive Sampling?



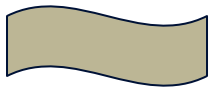
Oindrila Ghosh, Songjing Yan, Mandar Bokare, Upal Ghosh

Department of Chemical, Biochemical and Environmental Engineering,
University of Maryland Baltimore County

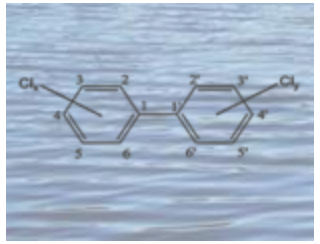
PASSIVE SAMPLING



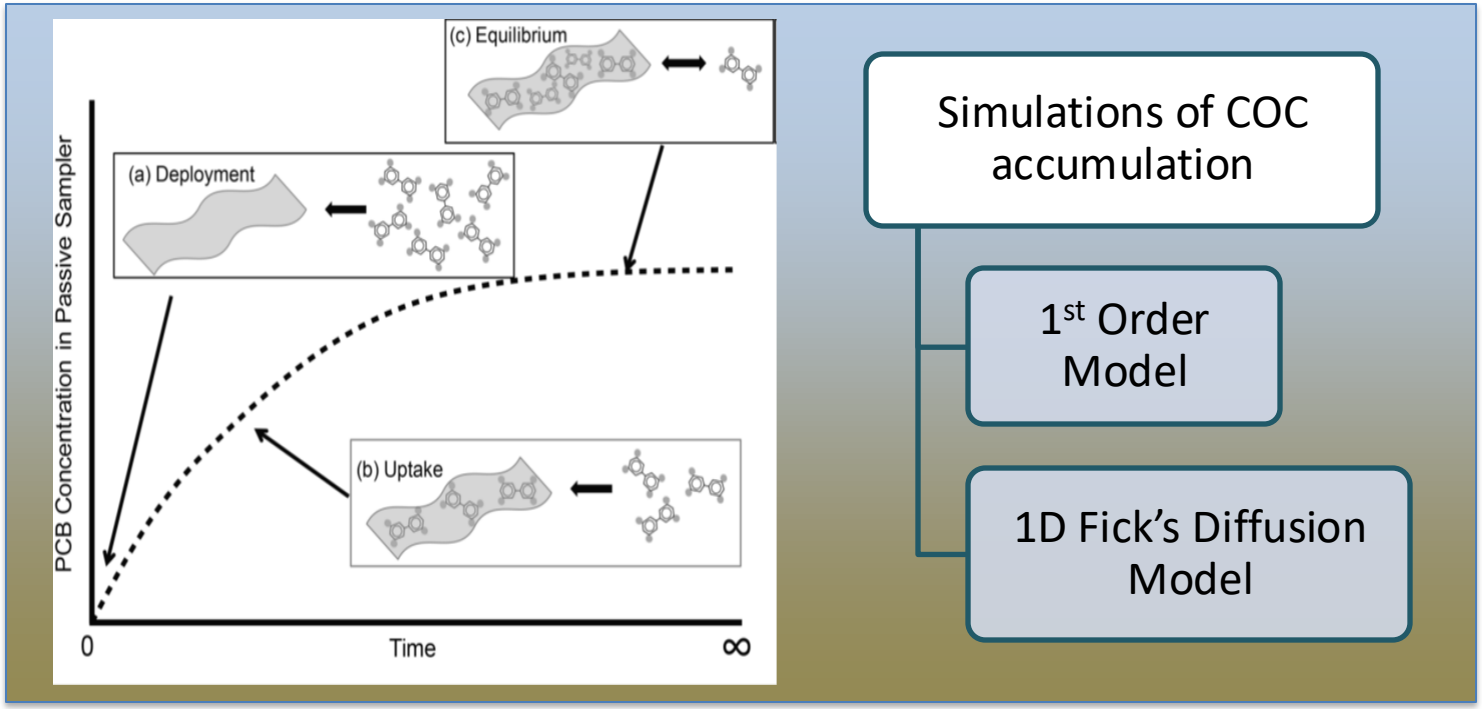
FREELY DISSOLVED CONCENTRATION (bioavailable)



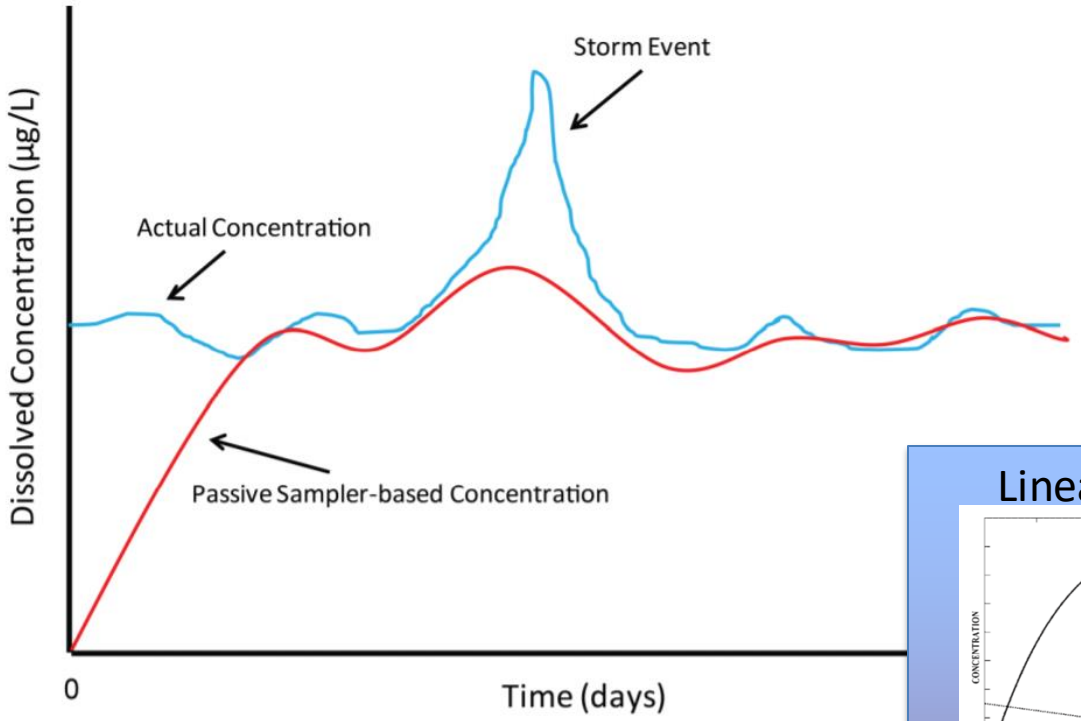
PASSIVE SAMPLER



Freely dissolved conc. of contaminant in water column/ interstitial water (ug/L) [Ghosh et al., 2014]



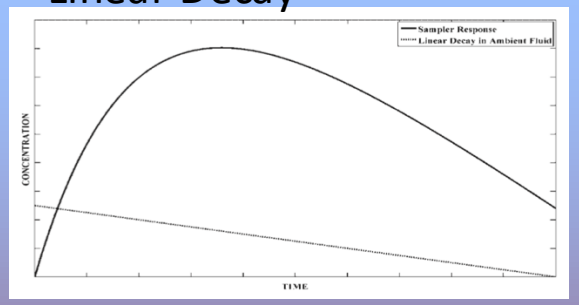
LITERATURE REVIEW & AIMS



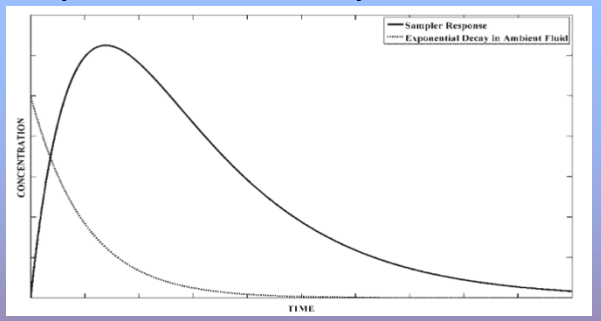
AIM

- In the real environment, water concentrations of these HOCs vary temporally.
- Important for ecological exposure assessment.
- **How well passive sampler concentrations represent the time-averaged concentration over an entire deployment period?**

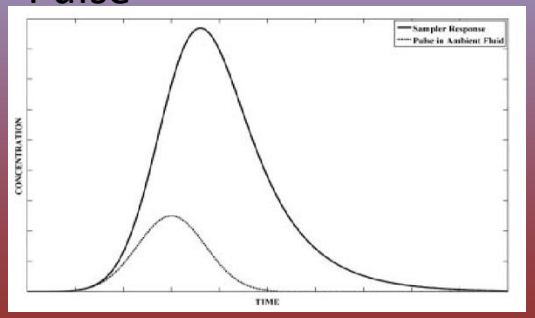
Linear Decay



Exponential Decay



Pulse

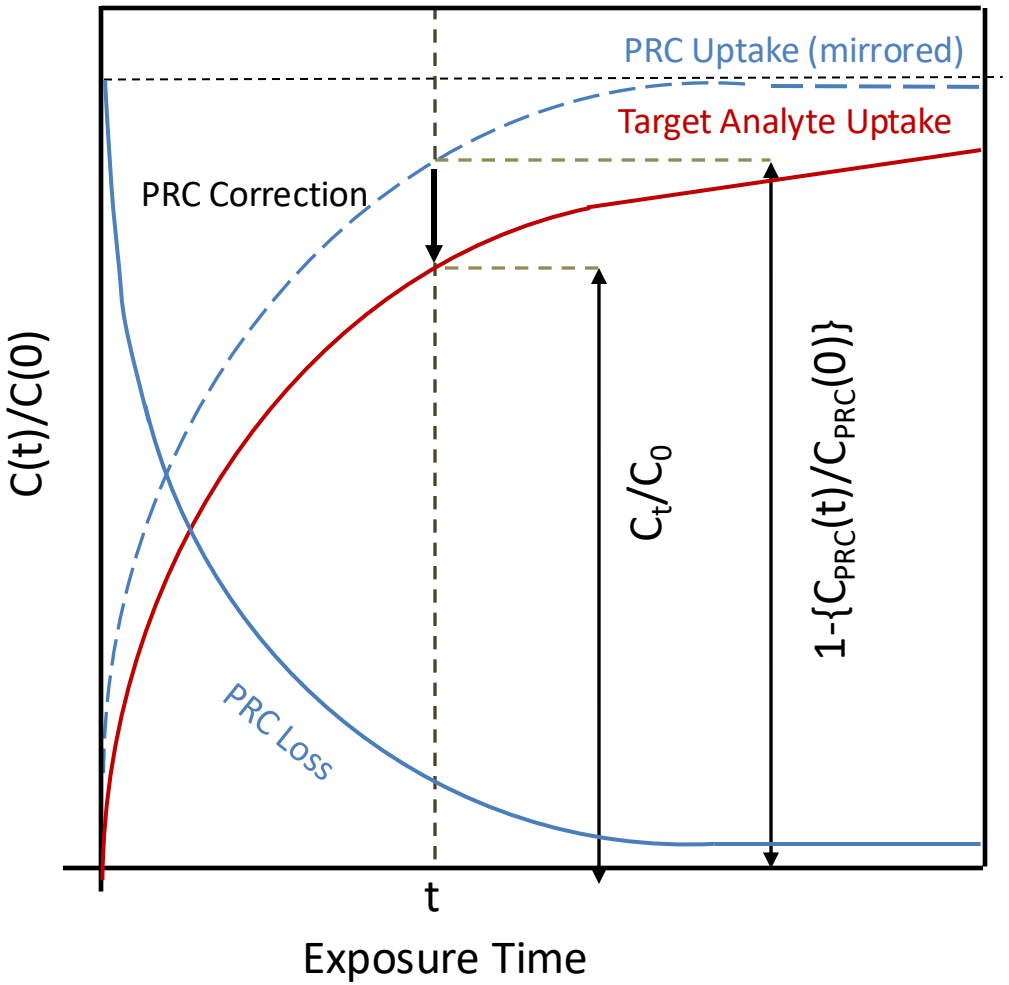


- Characteristic of ambient concentration
- Passive sampler-based water concentration (Analytical solution)

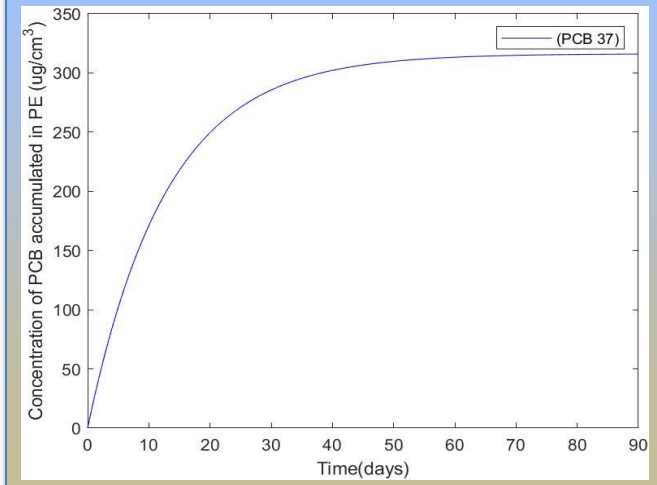
Hawker et al., 2009

METHODS: PRC CORRECTION

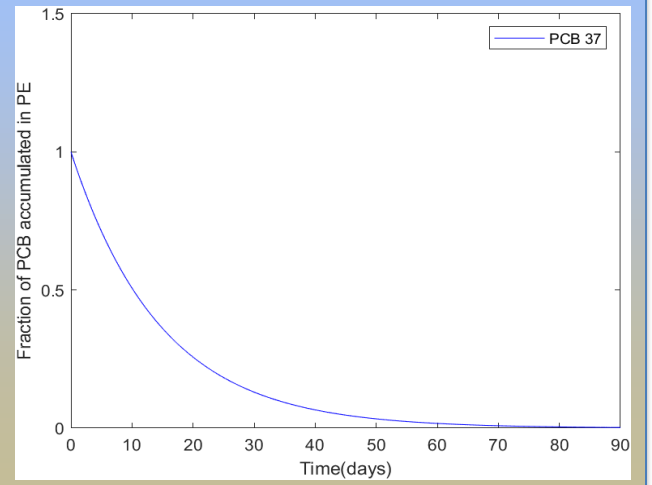
PERFORMANCE REFERENCE COMPOUND CORRECTION FOR EQUILIBRIUM



Gain Function = Actual Mass Gained



Loss Function = Fraction of Loss



$$Corrected\ Mass\ of\ PCB\ Uptake = \frac{Actual\ Mass\ Gained}{Fraction\ of\ Loss}$$

$$C_w = \frac{Corrected\ Mass\ of\ PCB\ Uptake}{K_{PEW}}$$

INITIAL CONDITIONS: Water concentration varies from 1ng/L to 0.1ng/L.

METHODS: FIRST ORDER & DIFFUSION MODELS

FIRST ORDER MODEL

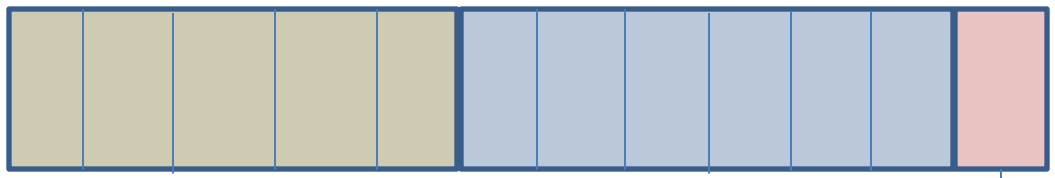
Governing Equation:

Calculation of Mass of PCB accumulated in PE (C_{PE})

$$\frac{dC_{PE}}{dt} = k_u C_w - k_e C_{PE}$$

Calculation of Mass of PCB accumulated in PE *at Equilibrium* (C_{PE_Eq})

$$C_{PE\_Eq} = C_{PE}/(1 - e^{-k_e T})$$



FICK'S DIFFUSION MODEL

Governing Equation: System of well mixed infinite water bath

Eq 1 $$\frac{\partial C_{PE}}{\partial t} = D_{PE}\frac{\partial^2 C_{PE}}{\partial x^2} \quad \text{for } -l < x < l$$

Eq 2 $$\frac{\partial C_W}{\partial t} = D_W\frac{\partial^2 C_W}{\partial x^2} \quad \text{for } -l > x > -(l+b) \text{ and } l < x < (l+b)$$

Boundary Conditions:

At the interface of the PE and water, the diffusive fluxes match so that mass is conserved

$$D_{PE}\frac{dC_{PE}}{dx} = D_W\frac{dC_W}{dx} \quad \text{for } x = l \text{ and } x = -l$$

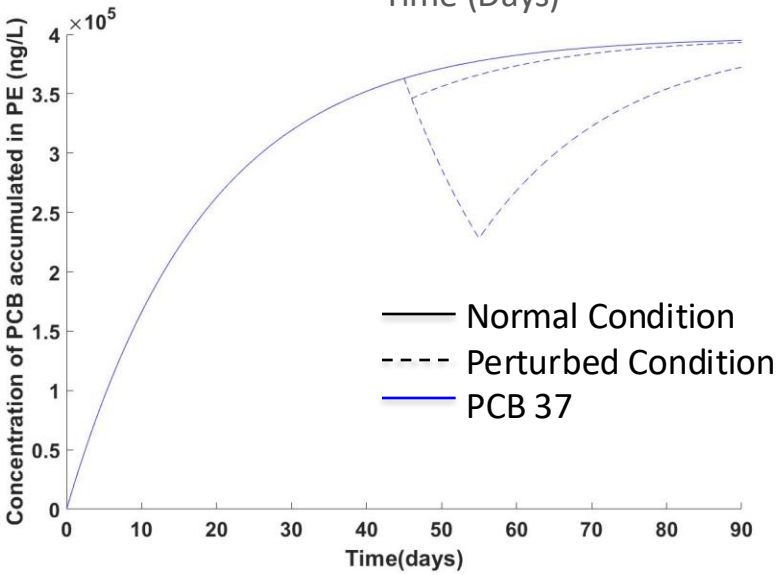
local equilibrium distribution

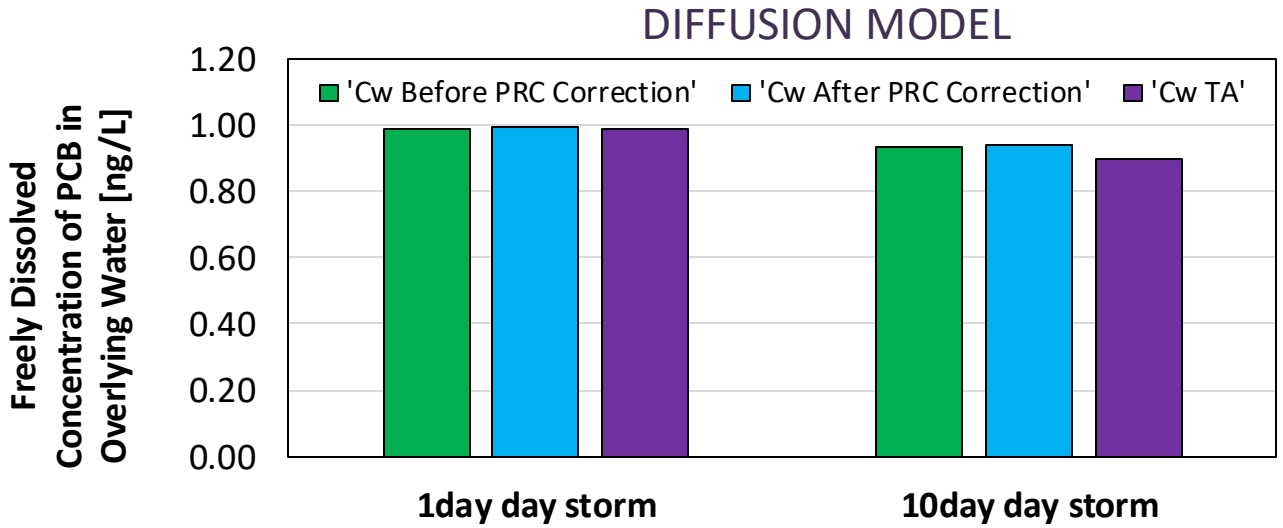
$$C_{PE} = K_{PEW}\,C_W \quad \text{at } x = l \text{ and } x = -l$$

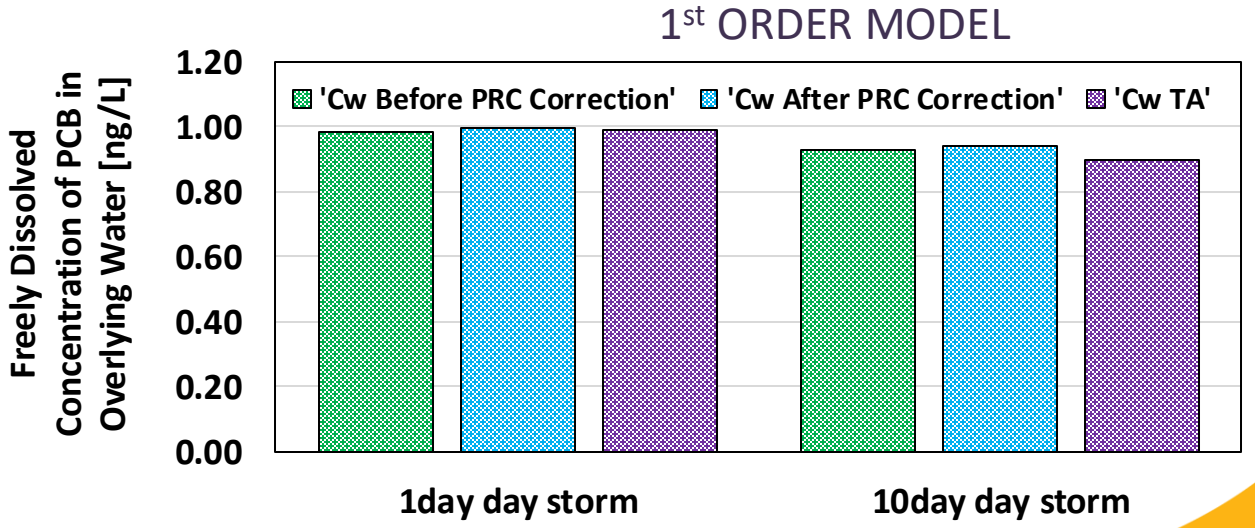
Eq 3

RESULTS

Impact of a 10-day long perturbation on the uptake of PCB 37

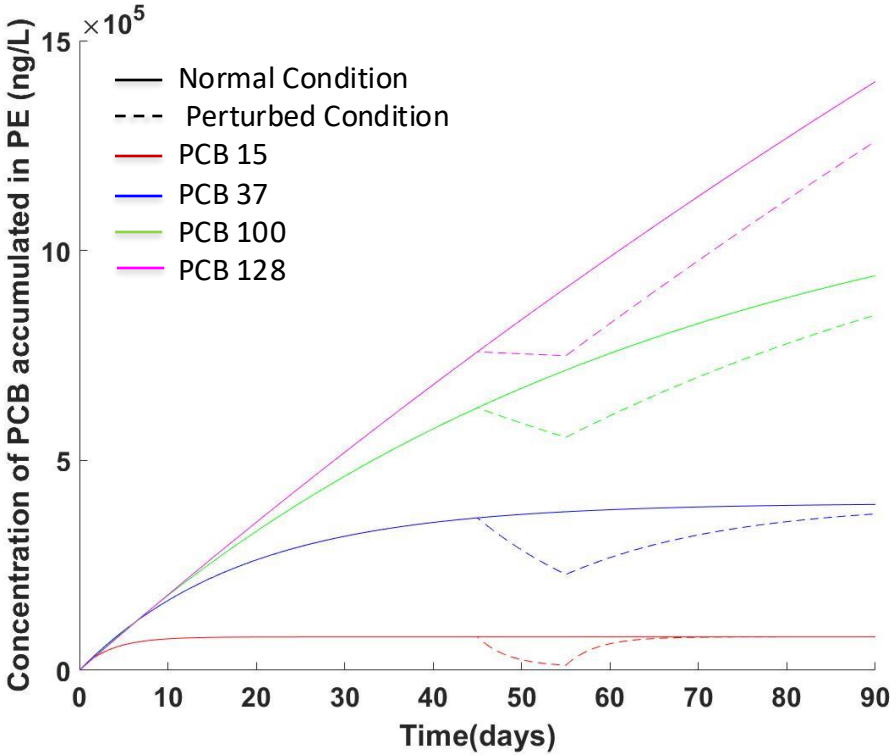




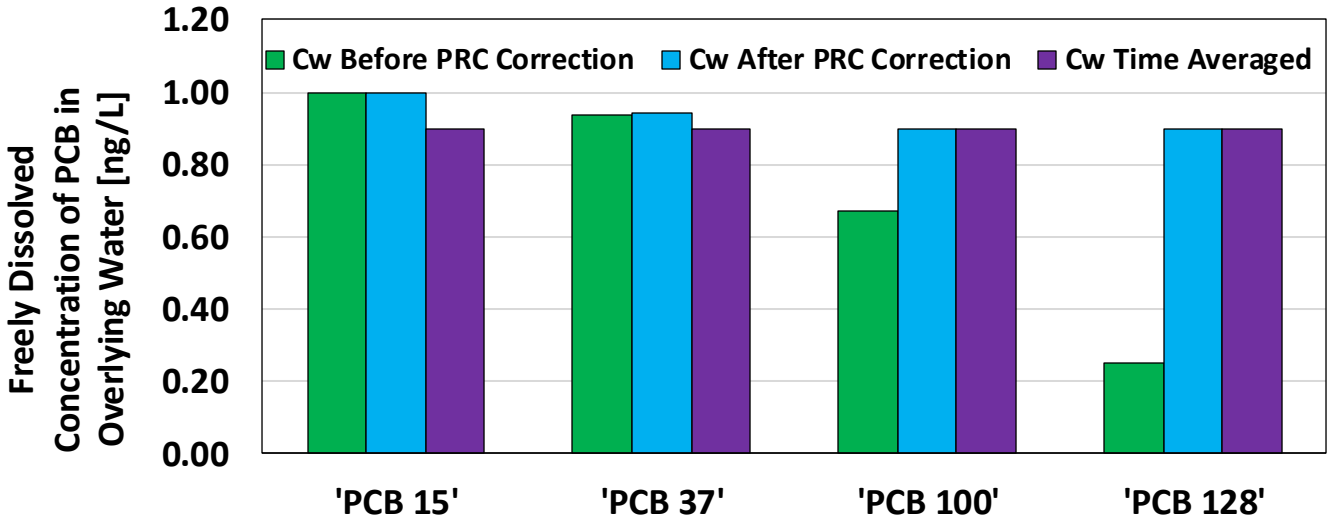


RESULTS

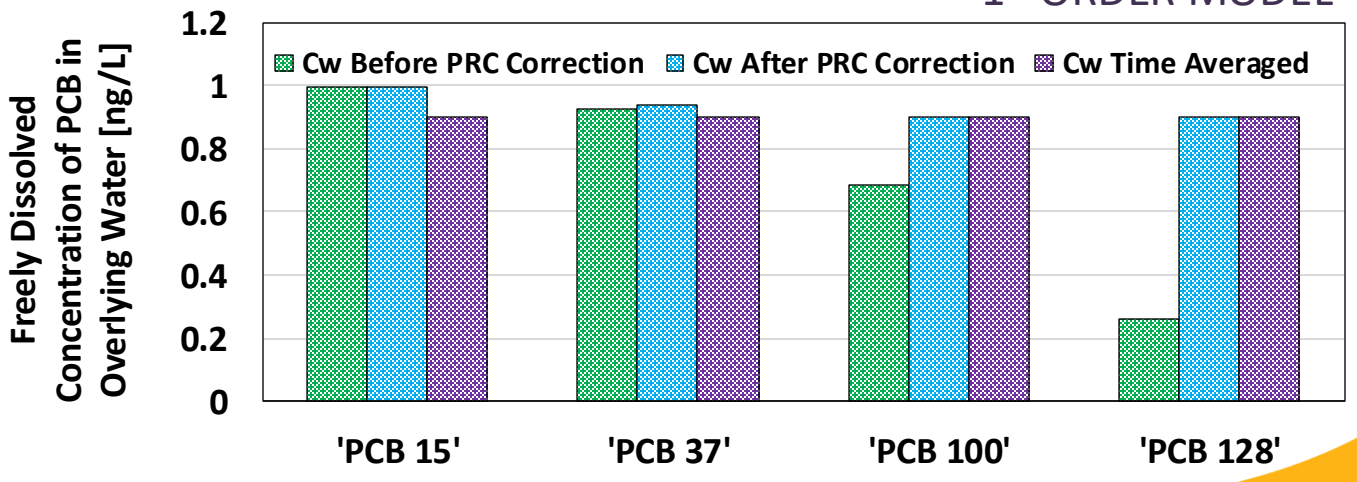
Effect of 10-day long perturbation on the uptake of different PCB homologs



DIFFUSION MODEL

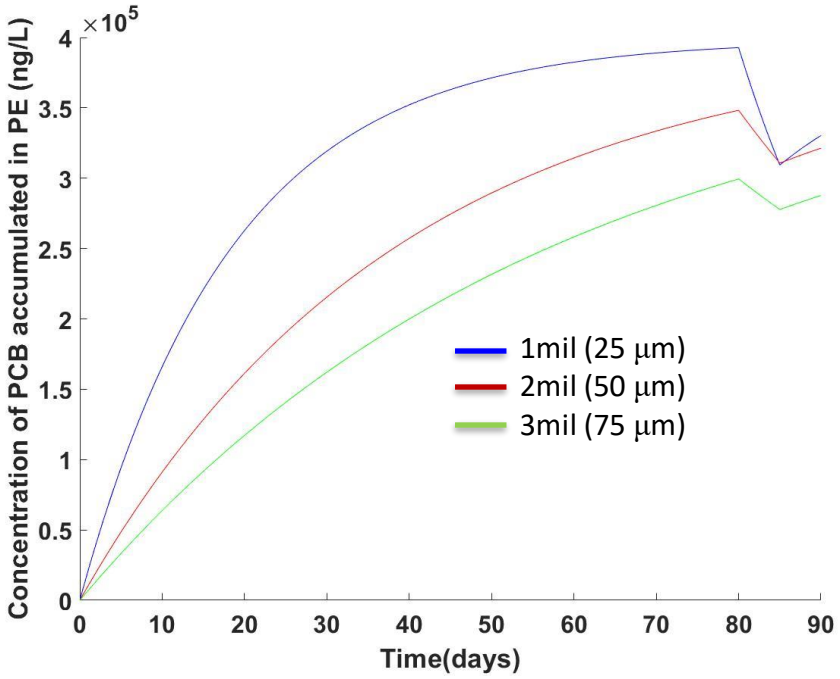


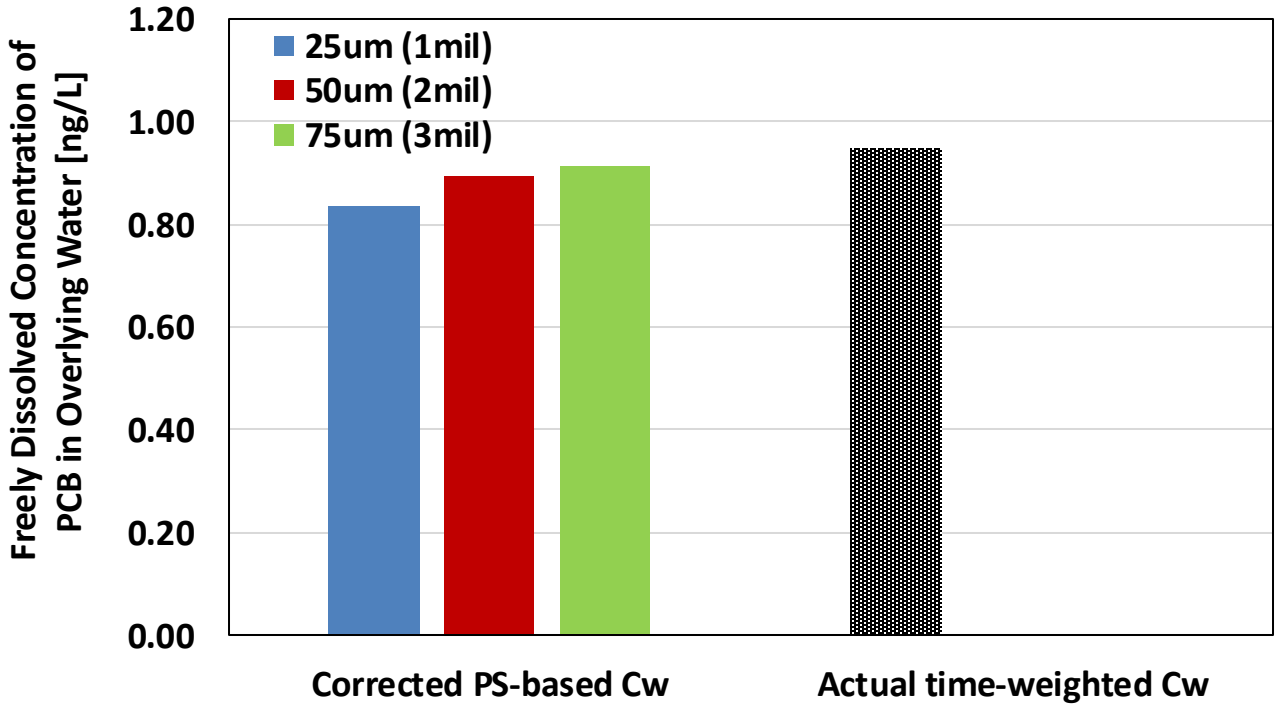
1st ORDER MODEL



RESULTS

Impact of various PE thickness on the uptake of PCB 37





CONCLUSION

- Is there a time period beyond which a perturbation in concentration is not captured in the passive sampling time-integration?

YES !

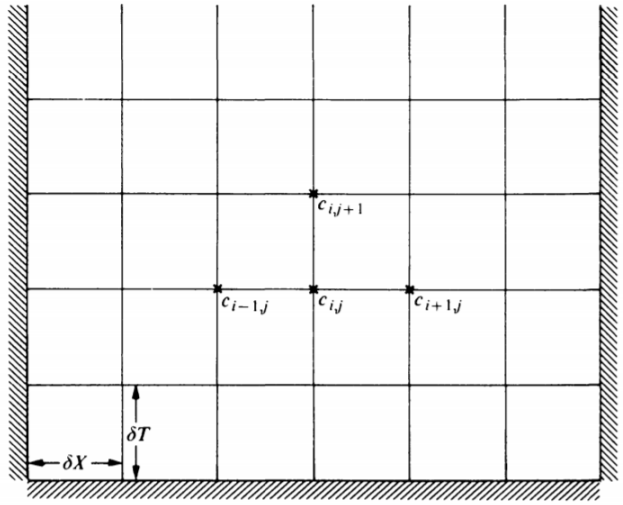
- Less hydrophobic = recovers from history of storm
  - Increasing hydrophobicity = returns truer Cw

- Thicker PE = returns truer Cw

Consistent.

THANK YOU

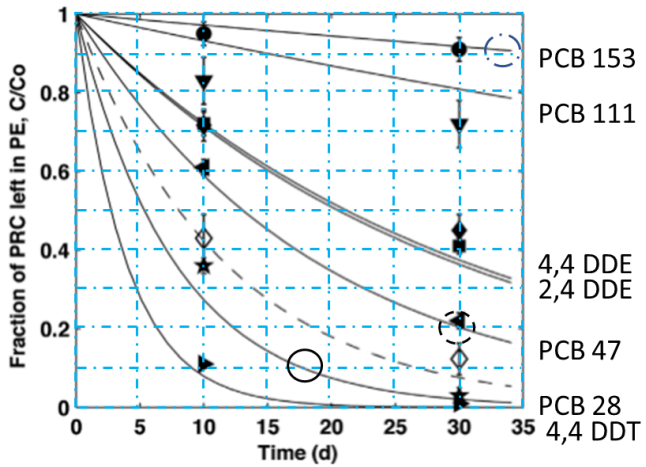
FINITE SOLUTION OF DIFFUSION MODEL



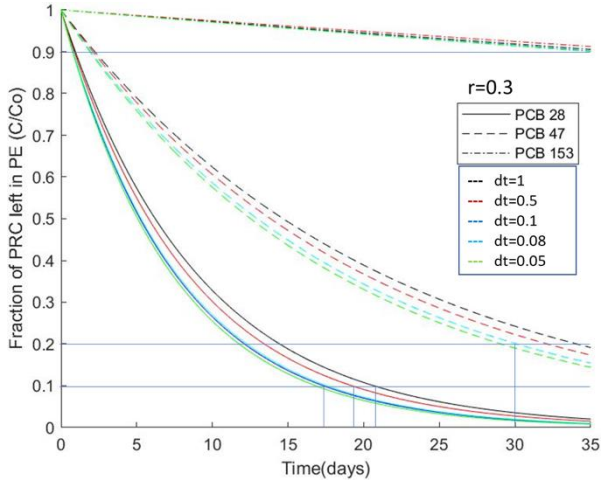
$$c_{i,j+1} = c_{i,j} + r(c_{i-1,j} - 2c_{i,j} + c_{i+1,j}),$$

$$r = \delta T/(\delta X)^2. \qquad r<0.5$$

Analytical solution in Tcacuic et al, 2015



Our Model

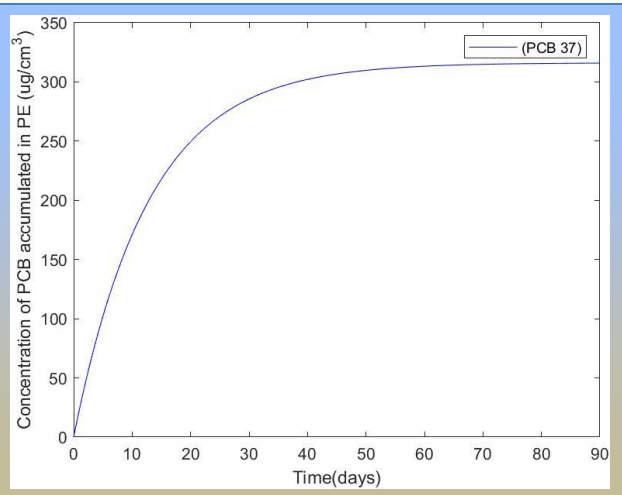


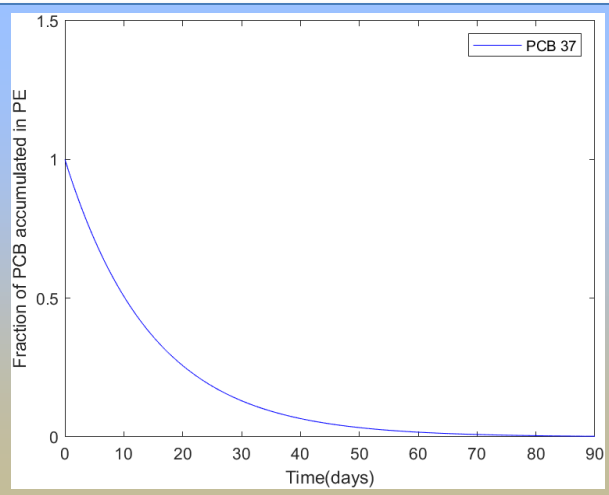
[wbl:0.02cm, 25um PE; Infinite Water Bath]

[r=0.3; dt=0.1s]

INITIAL CONDITIONS:

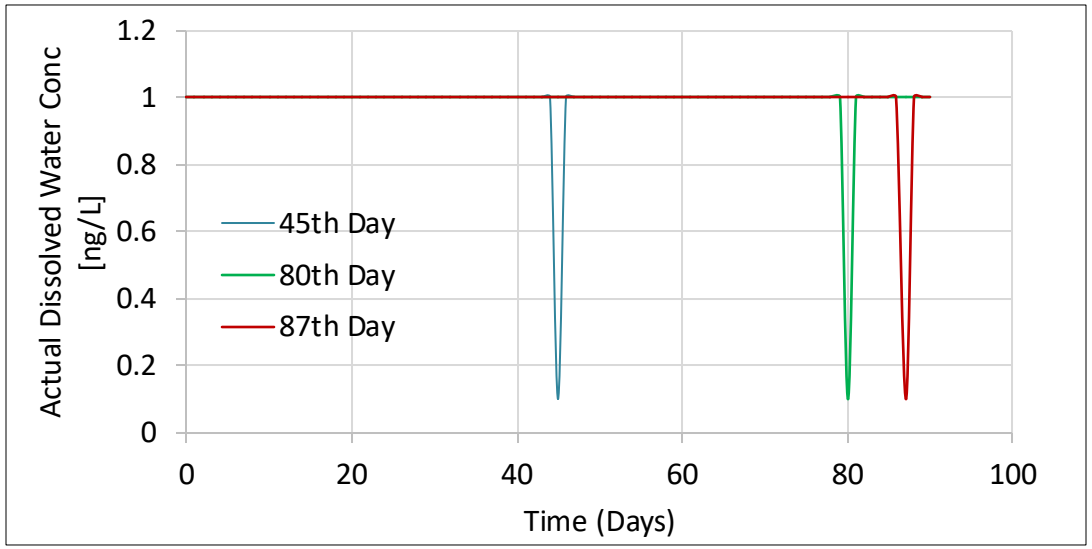
1. **NO STORM CONDITION**
   - Water: 1 ng/L
   - PE: 0 ng/L
2. **Storm**
   - Water: 0.1ng/L

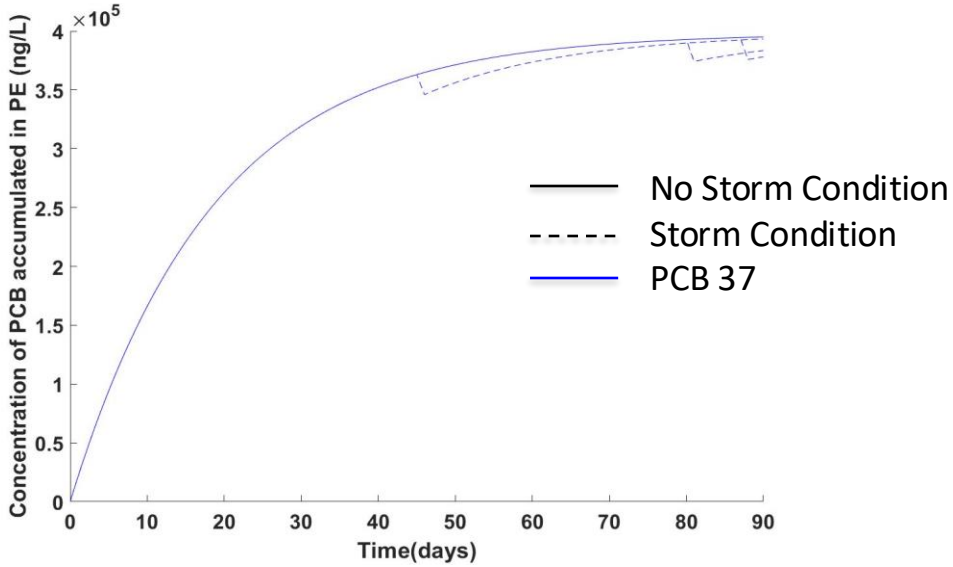


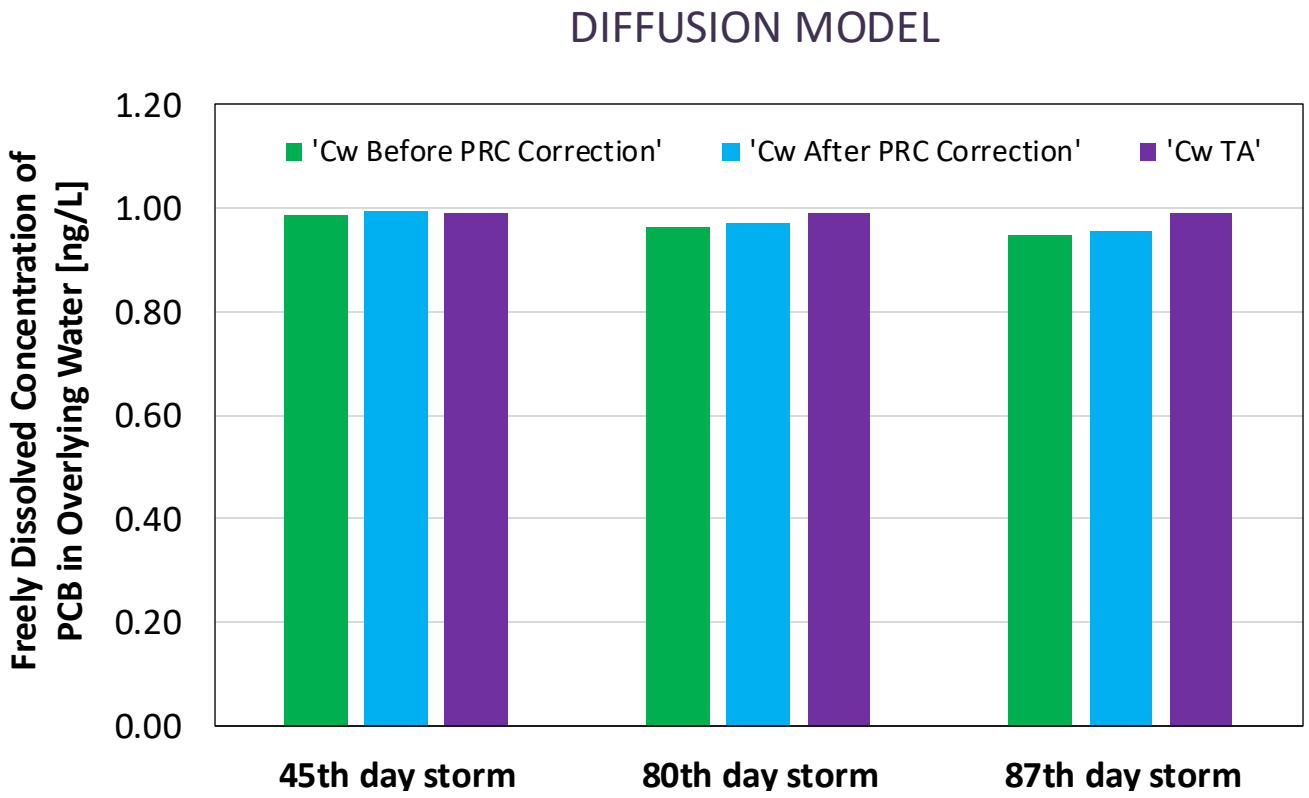


RESULTS

Impact of 1-day long storms on different days during the deployment period on the uptake of PCB 37

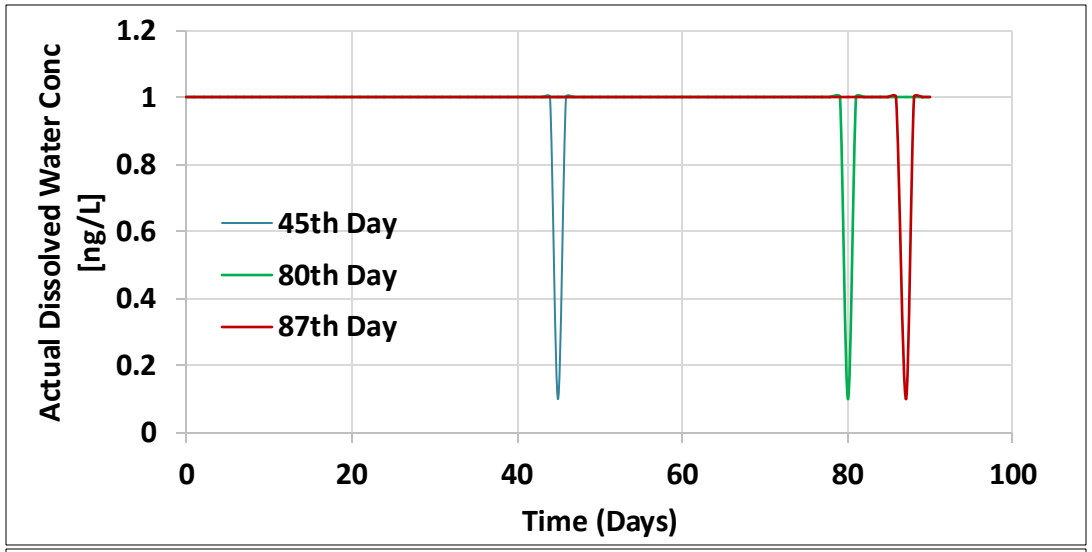


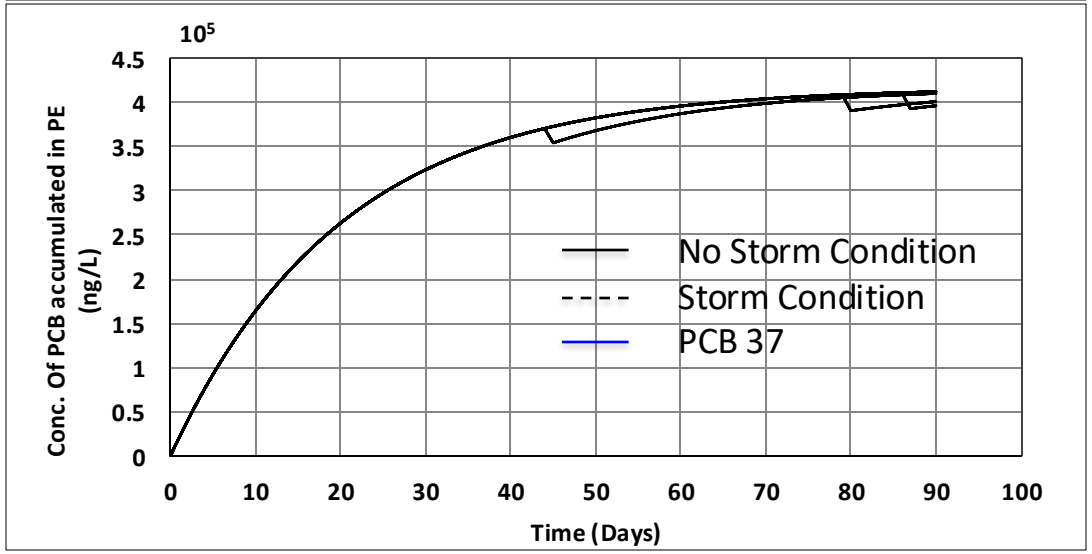




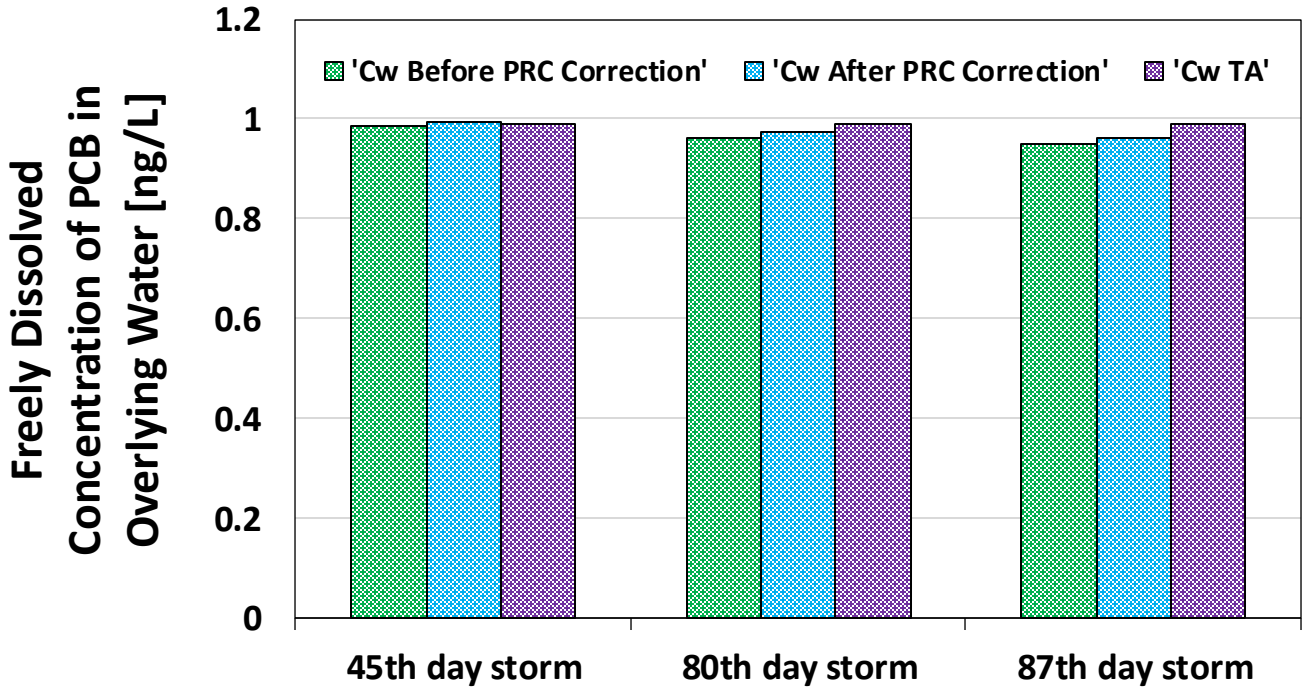
RESULTS

Impact of 1-day long storms on different days during the deployment period on the uptake of PCB 37



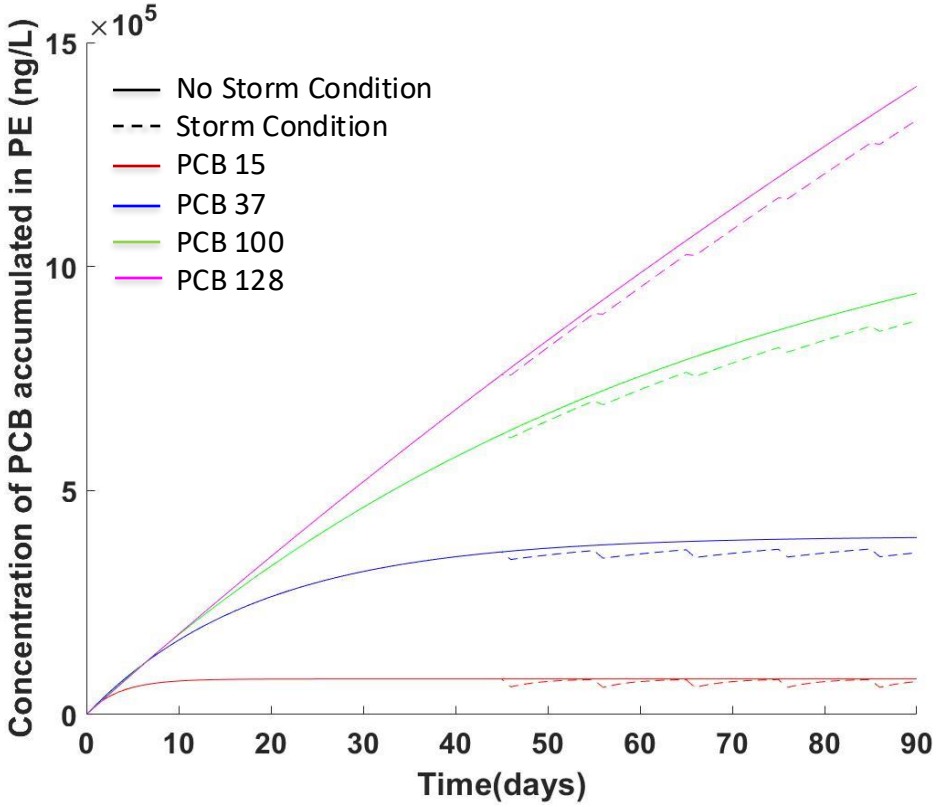


1st ORDER MODEL

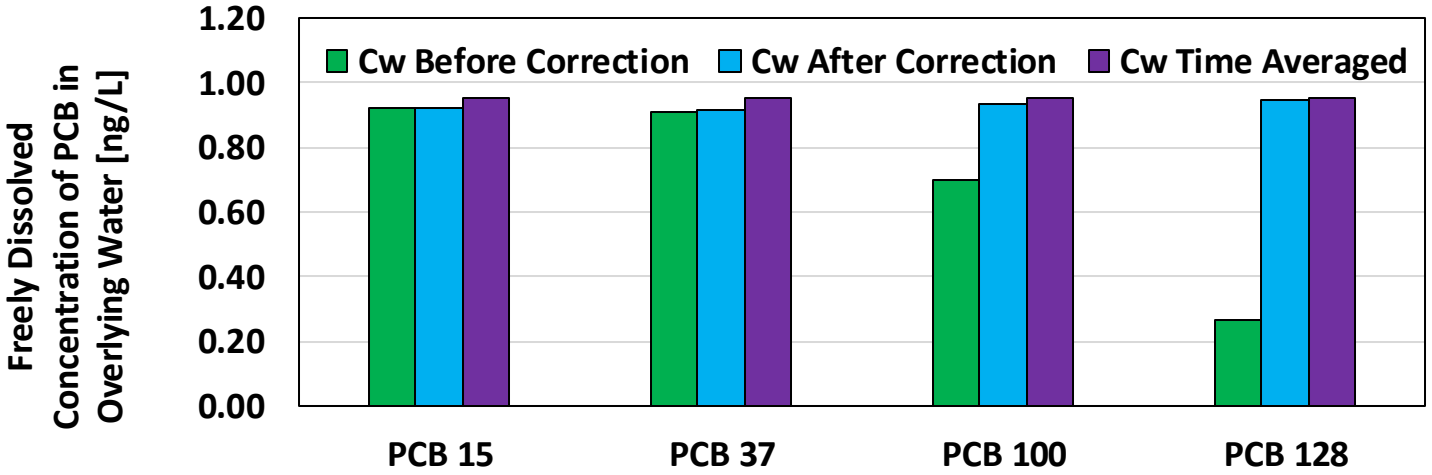


RESULTS

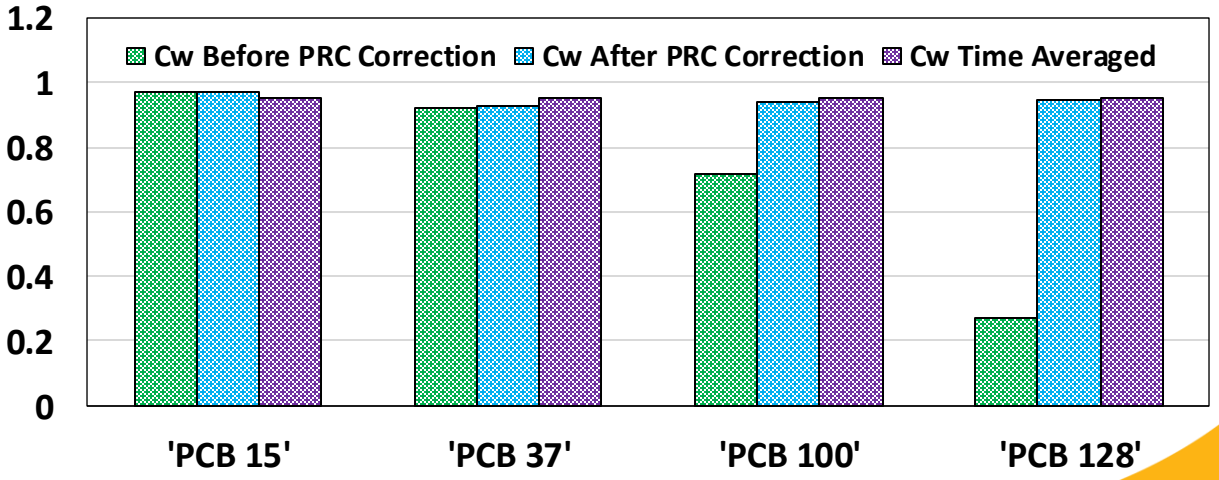
Impact of Periodic Storms on the Uptake of Various Homologs



DIFFUSION MODEL



1st ORDER MODEL



RESULTS

Impact of Varying Water Boundary Layer (WBL) Thickness on the Uptake of PCB 37