Phase equilibrium III:

Multi-phase equilibrium

Chemical potential

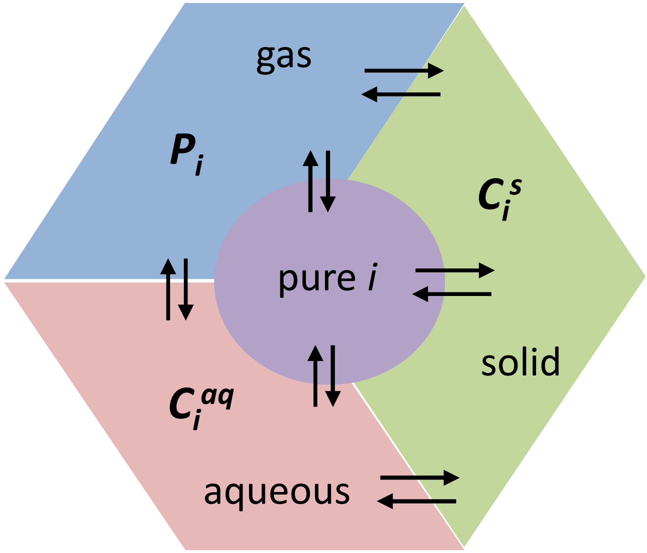
At equilibrium

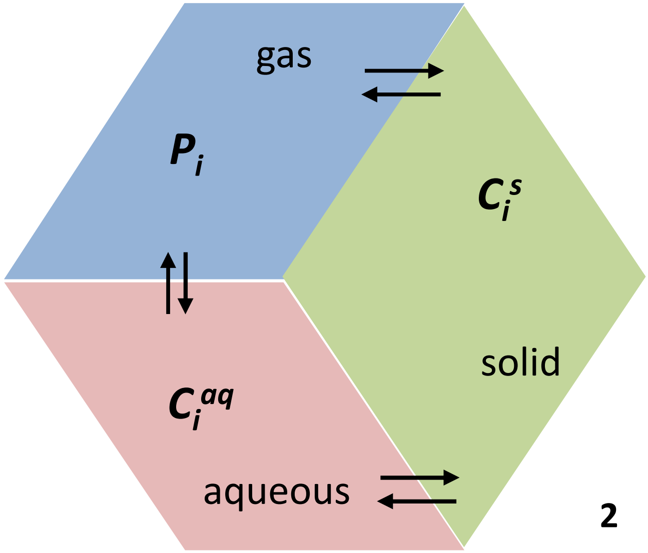
$$\mu_i{}^{pure} = \mu_i{}^{gas} = \mu_i{}^{s} = \mu_i{}^{aq}$$

(If pure phase exists)

$$\mu_i{}^{eq} = \mu_i{}^{gas} = \mu_i{}^{s} = \mu_i{}^{aq}$$

(If pure phase does not exist)





- μ is the <u>chemical potential</u> (energy) – difficult to measure
- **Chemical potential is related to activity**

  $\{i\}_{g,s,aq} \propto e^{\mu_i}$
- For gas phase, activity equals partial pressure expressed in atm

Fugacity – definition

Define the **fugacity** of a substance *i* in any phase to be equal to the **partial pressure of *i*** that is in equilibrium with the phase

at equilibrium

$f_i^{pure} = f_i^{s} = f_i^{aq} = f_i^{gas} = p_i^{sat}$ *(if pure phase exists)*

$f_i^{s} = f_i^{aq} = f_i^{gas} = p_i$ *(if pure phase does not exist)*

in other words, $\boldsymbol{f_i^j = f_i = p_i}$ ***for any phase** j*

- ***Why use p_i?***
  - Pressure is comprehensible & measurable
  - Gas phase behaves ideally – a good reference
    - $p_i \propto \{i\}$ for any substance at any reasonable p_i

Fugacity approach…

- **Enables predicting multi-phase equilibrium partitioning in a minimally complex fashion**

- Is applicable **in dilute systems when partitioning is linear among different phases**; suited for volatile compounds

Equilibrium partitioning review

- **Gas/water partitioning: Henry's law**

$$p_i = H_{pc} \times C_i^{aq} \qquad \text{or} \qquad C_i^{gas} = H_{cc} \times C_i^{aq}$$

- **Linear partitioning among water and any other phases**:

$$C_i^{oct} = K_{ow} \times C_i^{aq}$$

$$C_i^{biota*} = BCF \times C_i^{aq}$$

$$C_i^{s*} = K_p \times C_i^{aq}$$

$$\vdots$$

*Here, * is used for concentrations given in per mass basis; otherwise concentrations are in per volume basis*

Therefore we find:

$$C_i^{gas} = \boldsymbol{p_i} \times H_{cc}/H_{pc}$$

$$C_i^{aq} = \boldsymbol{p_i} \times 1/H_{pc}$$

$$C_i^{oct} = \boldsymbol{p_i} \times K_{ow}/H_{pc}$$

$$C_i^{biota*} = \boldsymbol{p_i} \times BCF/H_{pc}$$

$$C_i^{s*} = \boldsymbol{p_i} \times K_p/H_{pc}$$

$$\vdots$$

Applying fugacity approach

- **So:** if a system is at equilibrium and linear partitioning takes place, we can relate the concentration of a compound in any phase to partial pressure, or ***fugacity***
- **Now:** introduce ***Z value*** (fugacity capacity factor) to relate fugacity to concentration
- **Then:**

$$C_i^j = f_i Z_i^j$$

$$Moles_i^j = C_i^j V^j = f_i Z_i^j V^j$$

$$Moles_i^{total} = \sum_j Moles_i^j = \sum_j C_i^j V^j = f_i \sum_j Z_i^j V^j$$

*We find **Z** is in unit of e.g., [mol/m^3-atm]*

Z values for different phases

Recall

$$C_i^{gas} = \boxed{p_i} \times \boxed{H_{cc}/H_{pc}} \Rightarrow Z_i^{gas} = \frac{H_{cc}}{H_{pc}} = \frac{1}{RT}$$

$$C_i^{aq} = \boxed{p_i} \times \boxed{1/H_{pc}} \Rightarrow Z_i^{aq} = \frac{1}{H_{pc}}$$

$$C_i^{oct} = \boxed{p_i} \times \boxed{K_{ow}/H_{pc}} \Rightarrow Z_i^{oct} = \frac{K_{ow}}{H_{pc}}$$

Z values for solid phase – caution needed!

Note that concentrations in solid phase are typically expressed in *moles*$_{compound}$/*mass*$_{solid}$ or *mass*$_{compound}$/*mass*$_{solid}$

$$C_i^{s*} = K_p C_i^{aq}$$

C_i^{s*} per mass of solid (e.g., mol/kg)

K_p has a dimension of [(volume$_{water}$)/(mass$_{solid}$)] (e.g., m^3/kg)

- to use per volume basis unit for concentrations in solid phase:

$$C_i{}^s = \rho_s K_p C_i^{aq} = f_i \times \frac{\rho_s K_p}{H_{pc}} \quad \Rightarrow \quad Z_i^s = \frac{\rho_s K_p}{H_{pc}}$$

C_i^s per volume of solid (e.g., mol/m^3)

ρ_s = solid density (e.g., kg/m^3)

- alternatively, we may define ***Z**** for solids:

$$Z_i{}^{s*} = \frac{C_i{}^{s*}}{f_i} = \frac{K_p C_i^{aq}}{f_i} = \frac{K_p}{H_{pc}}$$

$Z_i{}^{s*}$ has a unit of e.g., mol/kg-atm

$$Moles_i{}^s = C_i{}^{s*} M^s = f_i Z_i{}^{s*} M^s$$

Applying fugacity approach

- **Our potential interest: how mass will be distributed among phases**
- **Need:**
  - Compartment volumes or masses
  - Equilibrium constants (Henry's constant, K_{ow}, K_p, etc.)

$$\boxed{\boldsymbol{Moles_i}^{\boldsymbol{total}} = \sum_{j} \boldsymbol{C_i}^{\boldsymbol{j}} \boldsymbol{V}^{\boldsymbol{j}} = \boldsymbol{f_i} \sum_{j} \boldsymbol{Z_i}^{\boldsymbol{j}} \boldsymbol{V}^{\boldsymbol{j}}}$$

If $Z_i{}^{j*}$ is obtained for any solid phase, substitute $Z_i{}^{j} V^{j}$ with $Z_i{}^{j*} M^{j}$ for that phase

- If we know $\boldsymbol{Moles_i}^{\boldsymbol{total}}$, we can calculate f_i and then determine $C_i{}^{j}$s and distributions among compartments
- If we know $\boldsymbol{f_i}$, we can calculate $Moles_i{}^{total}$ and then determine $C_i{}^{j}$s and distributions among compartments

Phase equilibrium IV:
Exercise

Mass partitioning between air & water

Q: A 1.000 L bottle is filled with 500.0 mL water. Then, 42.1 mg 1-hexene (MW: 84.2) is added. After sealing the bottle, it is left at 25°C until equilibrium between air and water. How will the 1-hexene mass partition between air and water in the bottle? If needed, use the following table.

Name	Formula	MW	Melting pt. (^{o}C)	Boiling pt. (^{o}C)	$-\log_{10}(p^{sat})$[1]	$-\log_{10}(C^{sat})$[1]
⋮	⋮	⋮	⋮	⋮	⋮	⋮
cyclohexane	C_6H_{12}	84.2	6.6	80.7	0.90	3.15
1-hexene	$\mathbf{C_6H_{12}}$	**84.2**	**-139.8**	**63.4**	**0.60**	**3.15**
benzene	C_6H_6	78.1	5.5	80.1	0.90	1.64
⋮	⋮	⋮	⋮	⋮	⋮	⋮

[1] p^{sat} = vapor pressure @ 25 ^{o}C, in atm

[2] C^{sat} = aqueous solubility @ 25 ^{o}C, in mol/L

Mass partitioning between air & water

From our discussion, we understand:

$$H_{pc} = \frac{p^{sat}}{C^{sat}}$$

$$= \frac{10^{-0.60}\ atm}{10^{-3.15}\ mol/L} = 10^{2.55}\ L - atm/mol$$

$$H_{cc} = \frac{H_{pc}}{RT} = \frac{10^{2.55}\ L - atm/mol}{24.47\ L - atm/mol} = 14.5$$

Recall that we have derived:

$$R_{g/aq} = \frac{M_g}{M_{aq}} = \frac{H_{cc} \times V_g}{V_{aq}}$$

$$= \frac{14.5 \times 500\ mL}{500\ mL} = 14.5$$

$$M_g = M_T \times \frac{R_{g/aq}}{1 + R_{g/aq}}$$

$$= 42.1\, mg \times \frac{14.5}{1 + 14.5} = \boldsymbol{39.4\, mg}$$

$$M_{aq} = M_T \times \frac{1}{1 + R_{g/aq}}$$

$$= 42.1\, mg \times \frac{1}{1 + 14.5} = \boldsymbol{2.7\, mg}$$

Fugacity approach

Q: Let’s work on a similar system as that for the previous example, but add an additional phase. A 1.000 L bottle is filled with 500.0 mL water and 20.0 mL octanol. How will 42.1 mg of 1-hexene added to the bottle partition among air, water, and octanol? Use the fugacity approach to answer. Calculate the 1-hexene fugacity (in atm) in the bottle.

* 1-hexene $\log_{10}K_{ow} = 3.40$

Fugacity approach

$$H_{pc} = 10^{2.55}\ L - atm/mol$$

$$K_{ow} = 10^{3.40}$$

Calculate Z values:

$$Z_{air} = \frac{1}{RT} = \frac{1}{(0.0821\ L - atm/mol - K) \times 298\ K}$$

$$= 0.0409\ mol/L - atm$$

** for any substance @ 25 ^{o}C & 1 atm, Z_{air} = 0.0409 mol/L-atm*

$$Z_{water} = \frac{1}{H_{pc}} = \frac{1}{10^{2.55}\ L - atm/mol} = 2.82 \times 10^{-3}\ mol/L - atm$$

$$Z_{oct} = \frac{K_{ow}}{H_{pc}} = \frac{10^{3.40}}{10^{2.55}\ L - atm/mol} = 7.08\ mol/L - atm$$

Now, construct a table as follows:

Phase (j)	**Volume (V^j in L)**	Z^j **(mol/L-atm)**	$Z^j \times V^j$ **(mol/atm)**	$Z^j \times V^j / \sum_j \left(Z^j \times V^j\right)$	**mass (mg)**
Air	0.480	0.0409	0.0196	0.120	**5.05**
Water	0.500	0.00282	0.00141	0.009	**0.36**
Octanol	0.020	7.08	0.142	0.871	**36.67**
Total			0.163	1.000	42.1

Recall $Moles^{total} = f \sum_j \left(Z^j V^j\right)$

$$f = \frac{Moles^{total}}{\sum_j (Z^j V^j)} = \frac{(42.1\ mg)/(84.2 \times 10^3\ mg/mol)}{0.163\ mol/atm}$$

$$= \mathbf{3.07 \times 10^{-3}}\ \boldsymbol{atm}$$

Fugacity approach – treating a solid phase

Q: Let's keep working on a 1.000 L bottle filled with multiple phases. Now, suppose 500.0 mL water and 100.0 g sediment is added to the bottle, leaving 450.0 mL as headspace. The sediment has an organic carbon content (f_{oc}) of 0.05, and it can be safely assumed that 1-hexene sorbed only to the organic fraction of sediment. How will 42.1 mg of 1-hexene added to the bottle partition among air, water, and sediment? Use the fugacity approach to answer. Calculate the 1-hexene fugacity (in atm) in the bottle.

Use the following K_{oc}-K_{ow} relationship:

$$K_{oc} = 0.63K_{ow}$$

Karickhoff et al. (1979); K_{oc} in L/kg

Fugacity approach – treating a solid phase

First, we need to obtain the sediment-water partition coefficient, K_p:

$$K_{oc}\ (in\ L/kg) = 0.63K_{ow} = 0.63 \times 10^{3.40}$$

$$= 1580\ L/kg$$

$$K_p = f_{oc}K_{oc} = 0.05 \times 1580\ L/kg$$

$$= 79.0\ L/kg$$

Now, let's get $Z_{sed}{}^*$:

$$Z_{sed}{}^* = \frac{K_p}{H_{pc}} = \frac{79.0\ L/kg}{10^{2.55}\ L - atm/mol} = 0.223\ mol/kg - atm$$

We already know Z values for air and water:

$$Z_{air} = 0.0409\ mol/L - atm, \qquad Z_{water} = 2.82 \times 10^{-3}\ mol/L - atm$$

The remaining procedure is the same as that for the previous question.

Phase (j)	**Volume or mass (V^j in L; M^j in kg)**	**Z^j or Z^{j*} (mol/L-atm)**	**$Z^j \times V^j$ or $Z^{j*} \times M^j$ (mol/atm)**	**$Z^j \times V^j / \sum_j (Z^j \times V^j)$**	**mass (mg)**
Air	0.450	0.0409	0.0184	0.437	**18.4**
Water	0.500	0.00282	0.00141	0.033	**1.4**
Sediment	0.100	0.223	0.0223	0.530	**22.3**
Total			0.0421	1.000	42.1

$$f = \frac{Moles^{total}}{\sum_j (Z^j V^j)} = \frac{(42.1\ mg)/(84.2 \times 10^3\ mg/mol)}{0.0421\ mol/atm}$$

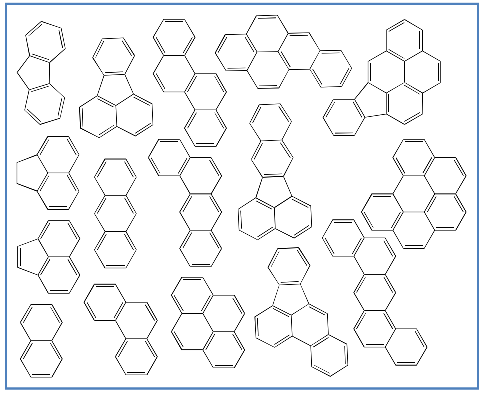
$$= \mathbf{1.19 \times 10^{-2}}\ \boldsymbol{atm}$$

Phase equilibrium application example:

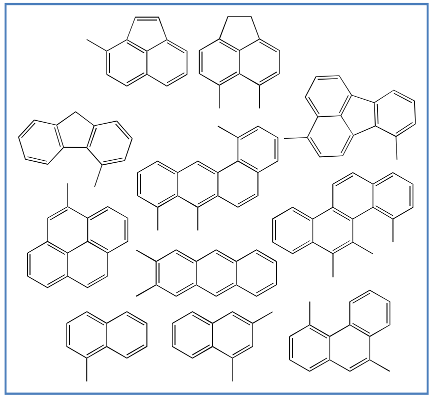
Passive Samplers

Hydrophobic organic contaminants (HOCs)

- **Low water solubility (log K_{ow} ≥ ~4)**
- **Major classes of HOCs of concern**
  - Polycyclic aromatic hydrocarbons (PAHs)
    - Generated by incomplete combustion
    - Found in urban areas (vehicles, etc.), thermal power plants, coal gasification plants, petroleum-related facilities, etc.
    - Main focus has been on parent-PAHs, but alkylated-PAHs can be also of interest (similar behavior and comparable toxicity)
    - Alkylated-PAHs dominant in petroleum (>90% of total)



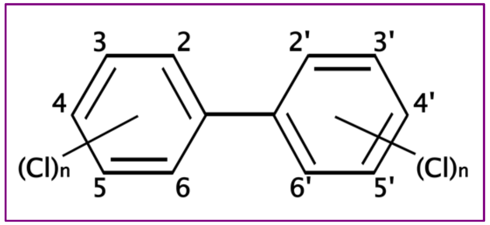
Parent-PAHs



Alkylated-PAHs

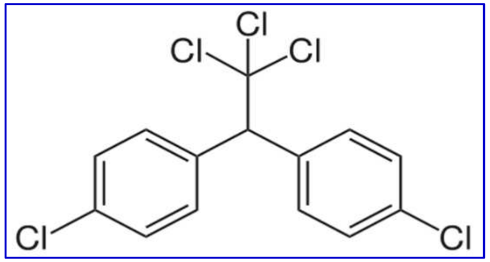
HOCs (cont’d)

#1



- Polychlorinated biphenyls (PCBs)
  - Used as insulator, plasticizer, flame retardants, etc.
  - Banned in the 1970s
  - But still of concern (highly persistent, endocrine disrupting)

#2

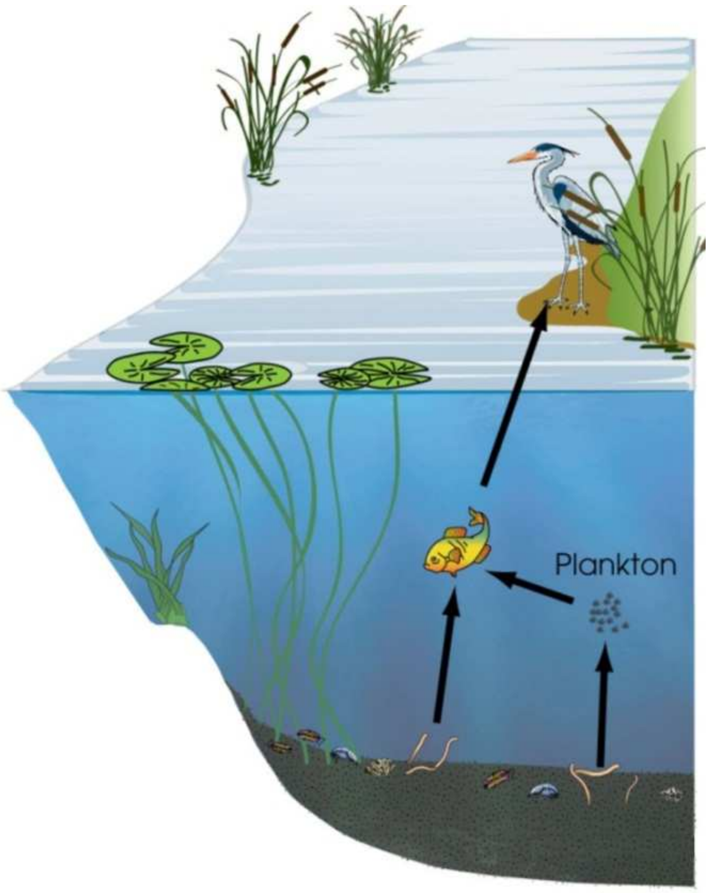


- Chlorinated pesticides
  - DDT and its metabolites
  - Methoxychlor, dieldrin, chlordane, toxaphene, …
  - Highly persistent

- **Significance of HOC contamination**
  - PCBs & PAHs are major risk-driving contaminants at contaminated sites in the U.S. (USEPA, 2005)
    - PCBs – one of risk drivers for 58% of sediment sampling stations in the U.S. where adverse effects are probable
    - PAHs – 8%

HOCs in sediment

- In the presence of an external contaminant source, sediment acts as a repository of HOCs
- When the external source is eliminated, sediment acts as an HOC source
- Enters the food chain either by sediment intake by benthic organisms or release to water column

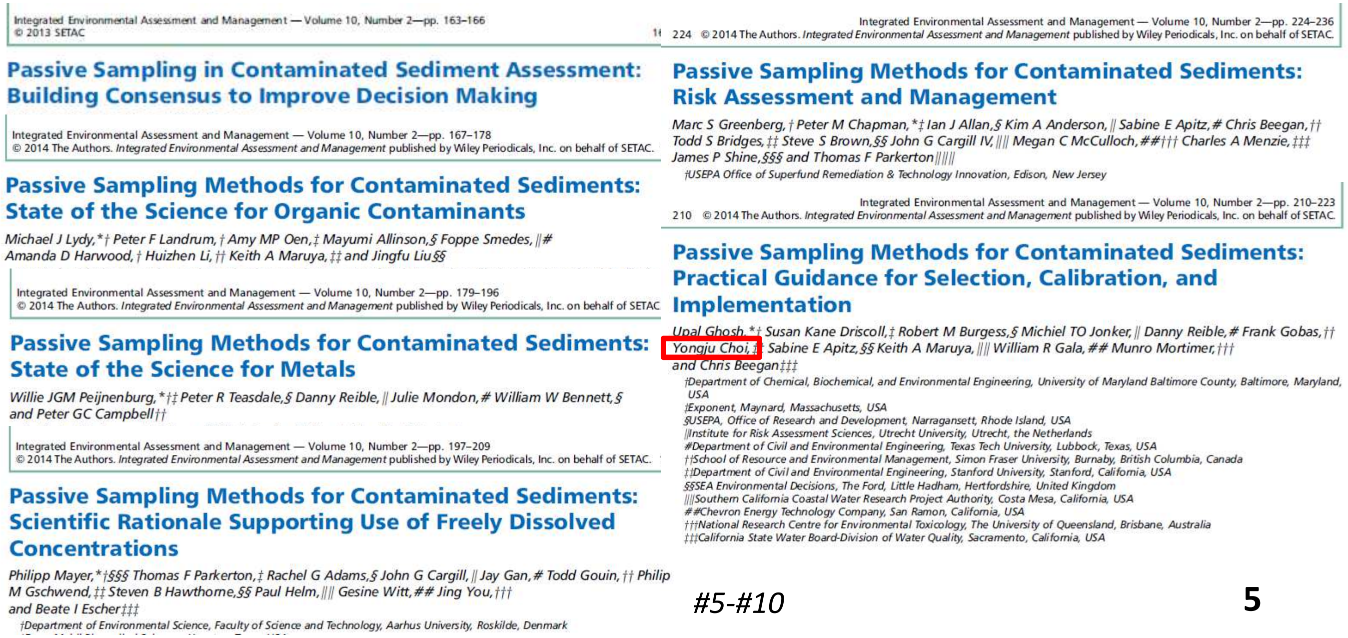


Ghosh et al. *ES&T Feature*, 2011[#3]

SETAC Workshop 2012

- Society of Environmental Toxicology & Chemistry (SETAC) 2012 Workshop
- 40+ faculty-level researchers
- Passive sampling guideline series in IEAM

#4



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Passive Sampling in Contaminated Sediment Assessment: Building Consensus to Improve Decision Making

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Passive Sampling Methods for Contaminated Sediments: State of the Science for Organic Contaminants

Michael J Lydy,† Peter F Landrum,† Amy MP Oen,‡ Mayumi Allinson,§ Foppe Smedes,‖# Amanda D Harwood,† Huizhen Li,†† Keith A Maruya,‡‡ and Jingfu Liu§§*

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Passive Sampling Methods for Contaminated Sediments: State of the Science for Metals

Willie JGM Peijnenburg,†‡ Peter R Teasdale,§ Danny Reible,‖ Julie Mondon,# William W Bennett,§ and Peter GC Campbell††*

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Passive Sampling Methods for Contaminated Sediments: Scientific Rationale Supporting Use of Freely Dissolved Concentrations

Philipp Mayer,†§§§ Thomas F Parkerton,‡ Rachel G Adams,§ John G Cargill,‖ Jay Gan,# Todd Gouin,†† Philip M Gschwend,‡‡ Steven B Hawthorne,§§ Paul Helm,‖‖ Gesine Witt,## Jing You,††† and Beate I Escher‡‡‡*

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Passive Sampling Methods for Contaminated Sediments: Risk Assessment and Management

Marc S Greenberg,† Peter M Chapman,‡ Ian J Allan,§ Kim A Anderson,‖ Sabine E Apitz,# Chris Beegan,†† Todd S Bridges,‡‡ Steve S Brown,§§ John G Cargill IV,‖‖ Megan C McCulloch,##††† Charles A Menzie,‡‡‡ James P Shine,§§§ and Thomas F Parkerton‖‖‖*

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Passive Sampling Methods for Contaminated Sediments: Practical Guidance for Selection, Calibration, and Implementation

Upal Ghosh,† Susan Kane Driscoll,‡ Robert M Burgess,§ Michiel TO Jonker,‖ Danny Reible,# Frank Gobas,†† Yongju Choi,‡‡ Sabine E Apitz,§§ Keith A Maruya,‖‖ William R Gala,## Munro Mortimer,††† and Chris Beegan‡‡‡*

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‖‖Southern California Coastal Water Research Project Authority, Costa Mesa, California, USA
##Chevron Energy Technology Company, San Ramon, California, USA
†††National Research Centre for Environmental Toxicology, The University of Queensland, Brisbane, Australia
‡‡‡California State Water Board-Division of Water Quality, Sacramento, California, USA

#5-#10

SETAC Workshop 2012 - Consensus

- **Consensus: absolute HOC concentration in sediment (C_{sed}) is NOT a valid indicator of HOC risk**
- **C_{free} as an alternative indicator**
  - **Freely-dissolved aqueous HOC concentration**: refers to the dissolved form of HOCs in water that is not associated with dissolved organic matter (DOM) or other species
  - Consensus: (at least) **a better indicator or HOC bioavailability than C_{sed}**
  - C_{free} is a direct indicator of “chemical activity” (or fugacity) in a multi-phase system
    - At equilibrium, bioaccumulation of HOCs would be proportional to chemical activity
  - Movement towards the use of C_{free} for regulation

C_{free} measurement by pore-water sampling

- Large volume requirement
  - C_{free} for HOCs is quite low → large volume is needed to ensure detectability
- Disturbance of the equilibrium during collection and analysis
- Difficulty to separate freely-dissolved species from DOM-bound species
- Labor and cost issues

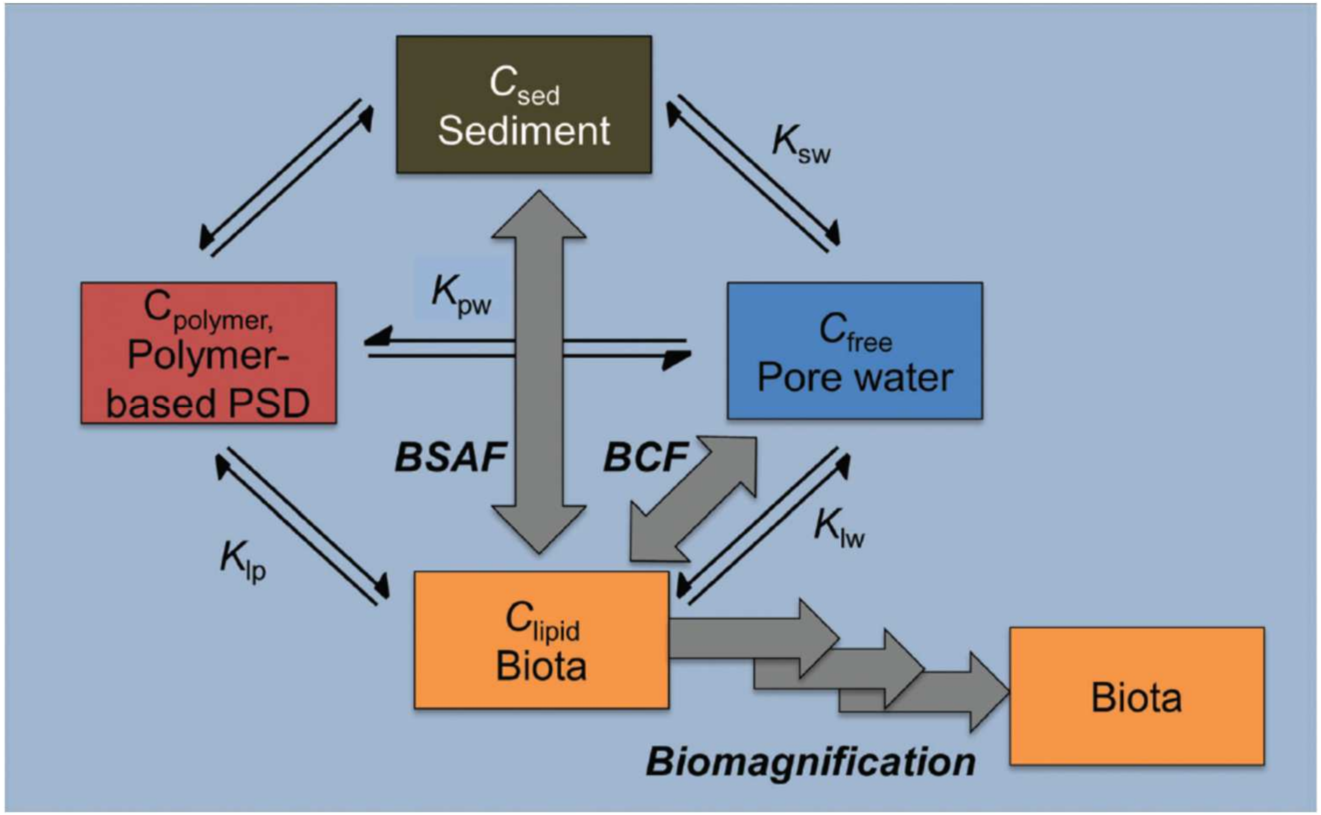
Comparison of a water sample before (right) and after (left) the DOM removal: DOM removed by a simplified (!!) flocculation technique developed by Ghosh et al. (2000, ES&T)[#11]

Now, the remaining steps are: liquid-liquid extraction (≥ 3 times) using hexane, moisture removal using sodium sulfate anhydrous, sample concentration under nitrogen stream, solvent exchange to cyclohexane (for PAHs), cleanup column, another sample concentration, and instrumental analysis

(estimated total labor time of ~ 10 hrs/sample, except for time required for sampling)

Alternative C_{free} measurement: Polymeric passive sampler

- Add a polymeric passive sampler into the sediment, collect the sampler after a certain period of exposure, determine $C_{polymer}$, and use the value to calculate C_{free}



#5

Polymeric passive samplers

- Low-density polyethylene (LDPE), polyoxymethylene (POM), polydimethylsiloxane (PDMS), …
- Linear HOC partitioning between polymer and water
- Large partitioning coefficient → can accumulate substantial amount of HOCs → remarkably enhanced sensitivity
- Inexpensive and easily available
- Easy to analyze HOC concentration (using a simple extraction technique and minimal cleanup requirements)
- Versatile applications: can fit into any scaffold

Application example (1)

Measurement of depth-profile of sediment pore-water HOC concentrations in the field

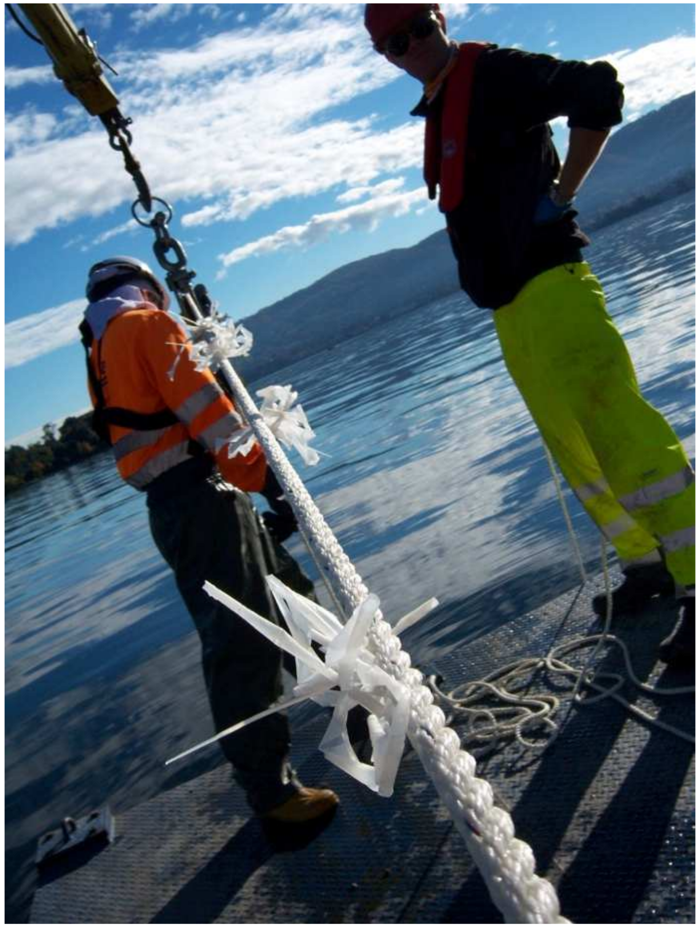
Application example (2)

Measurement of aqueous HOC concentration in the lab

Application example (3)

Sediment-water HOC flux measurement
(courtesy: Diana Lin, Stanford Univ.)

Application example (4)



Depth-profile of HOC C_{free} in the water column
(courtesy: Diana Lin, Stanford Univ.)

Sampling approaches (1)

- Equilibrium sampling
  - Exposure the passive sampler to the environment for a duration that is sufficient to achieve equilibrium for HOC partitioning
  - Applicable for laboratory deployment (or field deployment for relatively small/less hydrophobic contaminants)
  - Basic concept

$$C_{polymer,eq} = K_{polymer-water} \cdot C_{free}$$

$$\Rightarrow \quad C_{free} = C_{polymer,eq}/K_{polymer-water}$$

  - Ways to ensure that the exposure duration is sufficient for equilibrium
    - Collect passive samplers at different exposure durations [equilibrium if $C_{polymer} \neq f(time)$]
    - Deploy passive samplers with different thicknesses [equilibrium if $C_{polymer} \neq f(thickness)$]

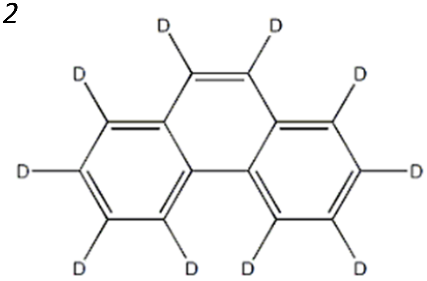
Sampling approaches (2)

- Non-equilibrium sampling
  - Equilibration time estimated for typical HOCs (e.g., PCBs, PAHs) in the field: months to years to decades
  - Equilibrium sampling not practically viable in most cases of field applications

- Current approach for non-equilibrium passive sampling
  - Use of "performance reference compounds (PRCs)"
    - PRCs: analytically non-interfering chemicals that are embedded in the passive sampler prior to environmental exposure (Ghosh, …, Choi et al., *IEAM*, 2014)

      ex) contaminant: phenanthrene → PRC: d10-phenanthrene

#12



d10-phenanthrene structure. All hydrogens are substituted with deuterons.

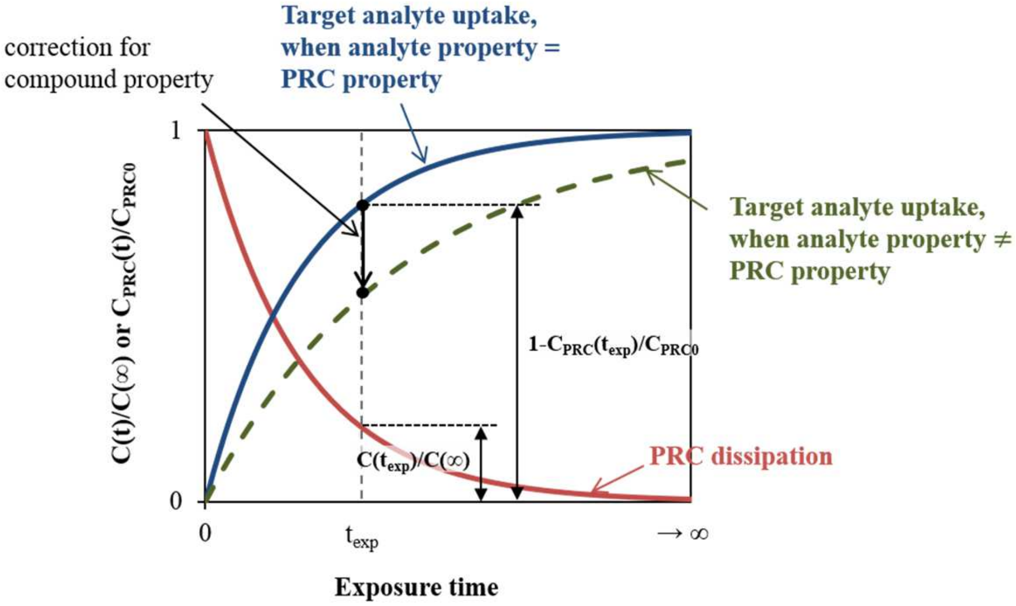
Sampling approaches (2) – cont'd

1) Impregnate passive sampler with PRCs

2) Expose the sampler to the target media

3) After exposure, analyze both the target contaminant and PRC concentration in the sampler [$C(t_{exp})$, $C_{PRC}(t_{exp})$]

4) Calculate the fraction of the PRC released out of sampler [$1\text{-}C_{PRC}(t_{exp})/C_{PRC0}$]



5) Calculate the fraction of the target contaminant accumulated in the sampler compared to the equilibrium value [$C(t_{exp})/C(\infty)$]

6) Calculate target contaminant concentration at equilibrium [$C(\infty)$]

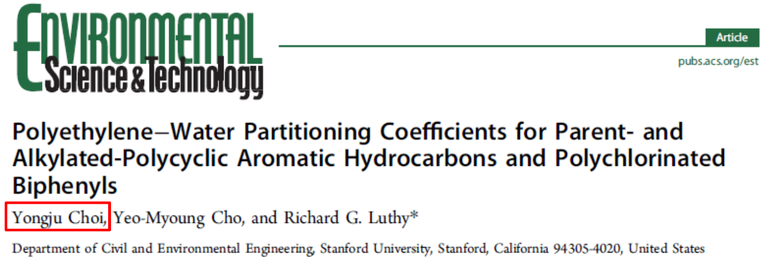
7) Obtain C_{free} [$= C(\infty)/K_{polymer\text{-}water}$]

Addt’l note for non-eq. sampling

- PRC method reasonably works for most situations, but has been criticized by some researchers
- Basic assumption of the PRC method: “isotropic exchange kinetics”
    - The rate of PRC dissipation from the sampler is expressed in exactly the same way as the rate of target contaminant accumulation by the sampler
- Experiments show that the isotropic exchange kinetics assumption may not hold
    - Because of the resistance of a PRC for dissipation from the sampler
    - More significantly, because of the resistance of a target contaminant for desorption from the sediment

Some relevant publications

#13



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Polyethylene–Water Partitioning Coefficients for Parent- and Alkylated-Polycyclic Aromatic Hydrocarbons and Polychlorinated Biphenyls

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Passive Sampling Methods for Contaminated Sediments: Practical Guidance for Selection, Calibration, and Implementation

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Non-equilibrium passive sampling of hydrophobic organic contaminants in sediment pore-water: PCB exchange kinetics

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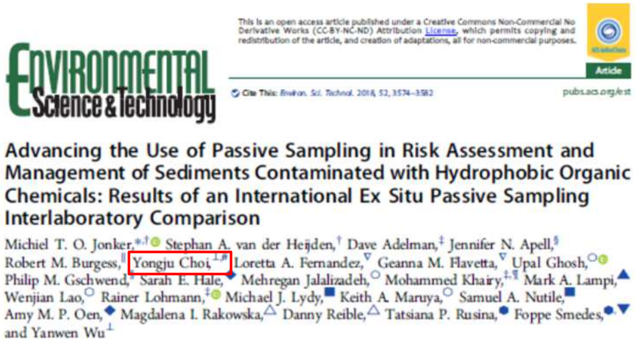

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Advancing the Use of Passive Sampling in Risk Assessment and Management of Sediments Contaminated with Hydrophobic Organic Chemicals: Results of an International Ex Situ Passive Sampling Interlaboratory Comparison

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