United States Environmental Protection Agency

University of Minnesota
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A stochastic framework for addressing chemical partitioning and bioavailability in contaminated sediment assessment and management

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Outline

1) Background & Motivation

2) Approach

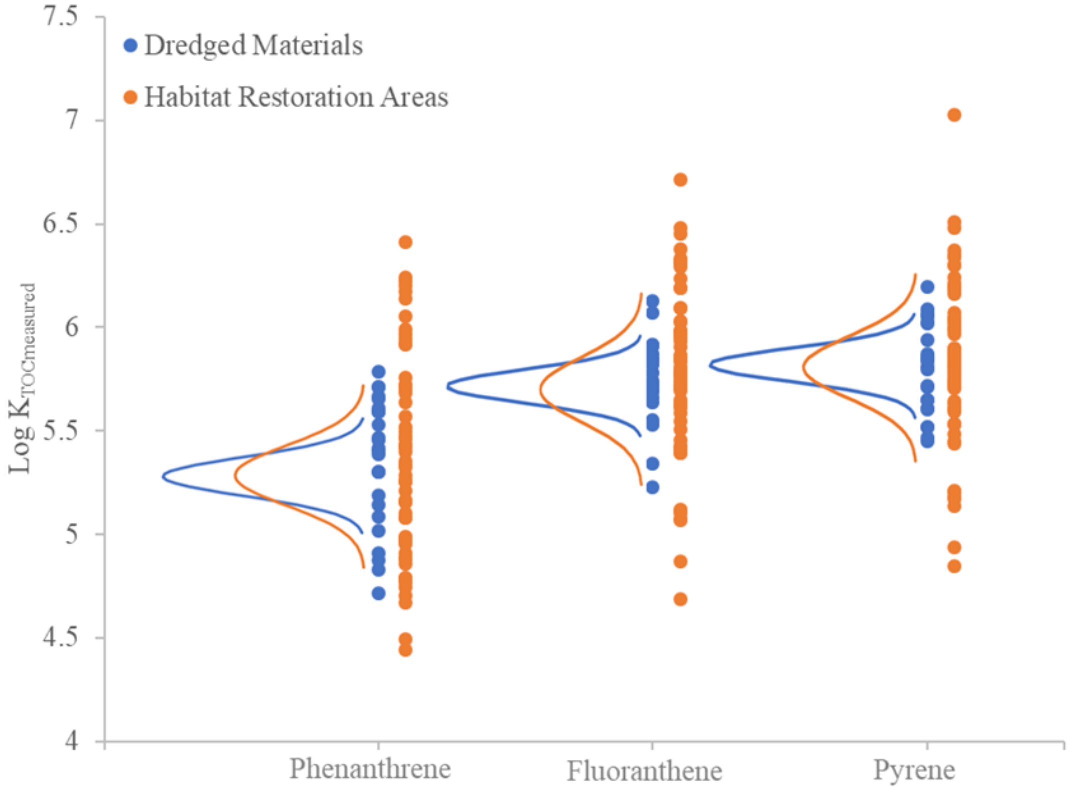
3) Results

4) Conclusions

Background & Motivation

Log K_{TOC}

$$= \frac{C_{total_{TOC}}}{C_{free}}$$



Which K_{TOC} value do you use?

- C_{free}: risk
- C_{total}: Cleanup remediation & restoration goals

[1]https://www.quora.com/What-is-the-difference-between-caking-and-non-caking-coal [2]http://www.modifiedcoaltarpitch.com/sale-10003249-black-carbon-coal-tar-pitch-58-coking-value-for-prebaked-anode-cells.html

Goals of the Bioavailability Ratio (BR)

Addresses two key points:

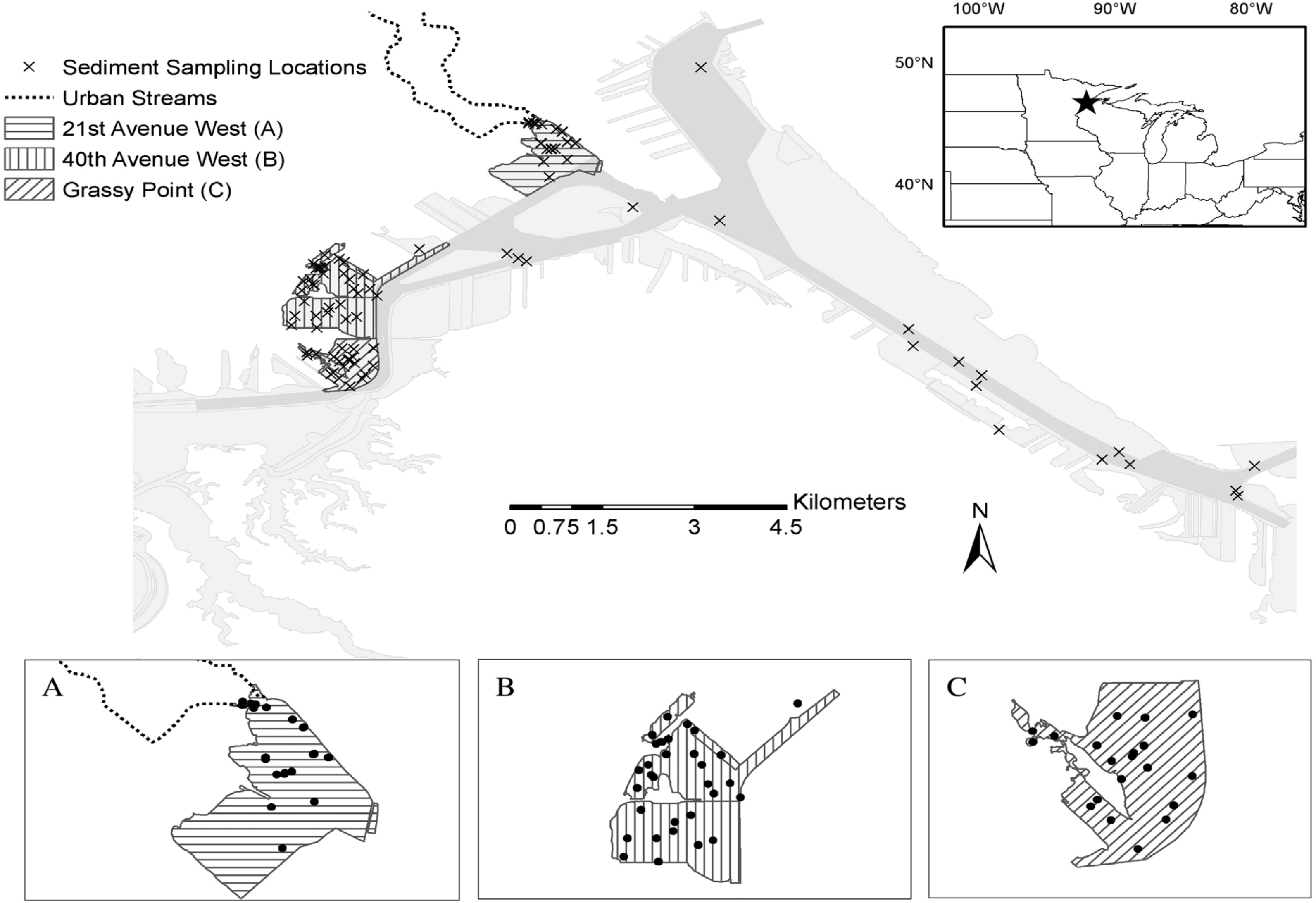
1) Provides a formal way of quantifying variance in contaminant partitioning

2) Translating bioavailability among phases relevant for contaminant characterization: C_{free}, C_{total}, C_{lipid}

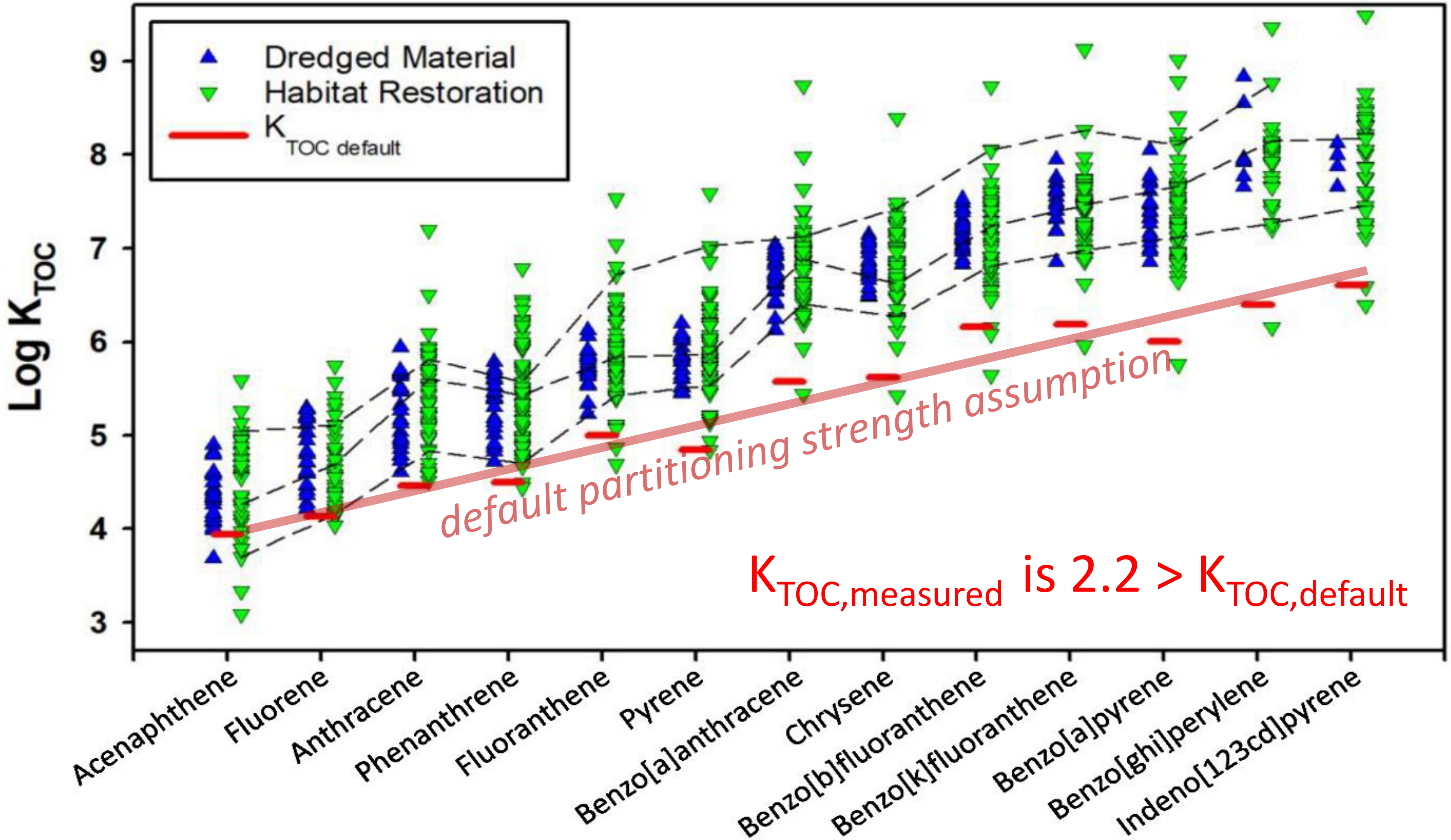
Approach

SPME-derived K_{TOC} Values

- Paired C_{total} & C_{free}
- St. Louis River Estuary, Duluth, MN
- 85 sediments
  - Habitat restoration areas (**HRA**): 62
  - Dredged materials (**DM**): 23



K_{TOC} Variability



$K_{TOC,measured}$ is 2.2 > $K_{TOC,default}$

Bioavailability Ratio

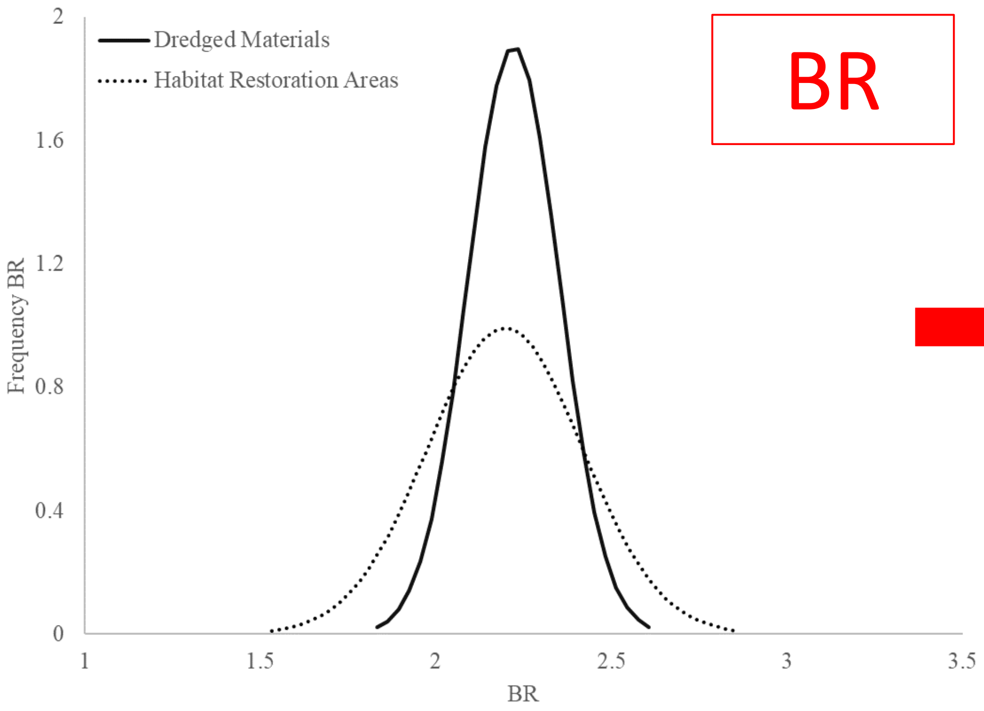
- PAHs present in the environment as mixtures
- Toxic Unit (TU) approach aggregates exposure and potency of PAHs
  - $TU_i = \sum_{j=1}^{n} \frac{C_{free_{i,j}}}{FCV_j}$
- Bioavailability ratio (BR): ***potency-weighted net partitioning strength***

$$BR_i = \boxed{\frac{\Sigma ESBTU_j}{\Sigma IWTU_j}} = \frac{\Sigma\left(\frac{\left(\frac{C_{total,TOC_j}}{K_{TOC,default_j}}\right)}{FCV_j}\right)}{\Sigma\left(\frac{\left(\frac{C_{total,TOC_j}}{K_{TOC,measured_j}}\right)}{FCV_j}\right)}$$

$K_{TOC,default}$ as "reference quantity"

$K_{TOC,measured}$ based on observations

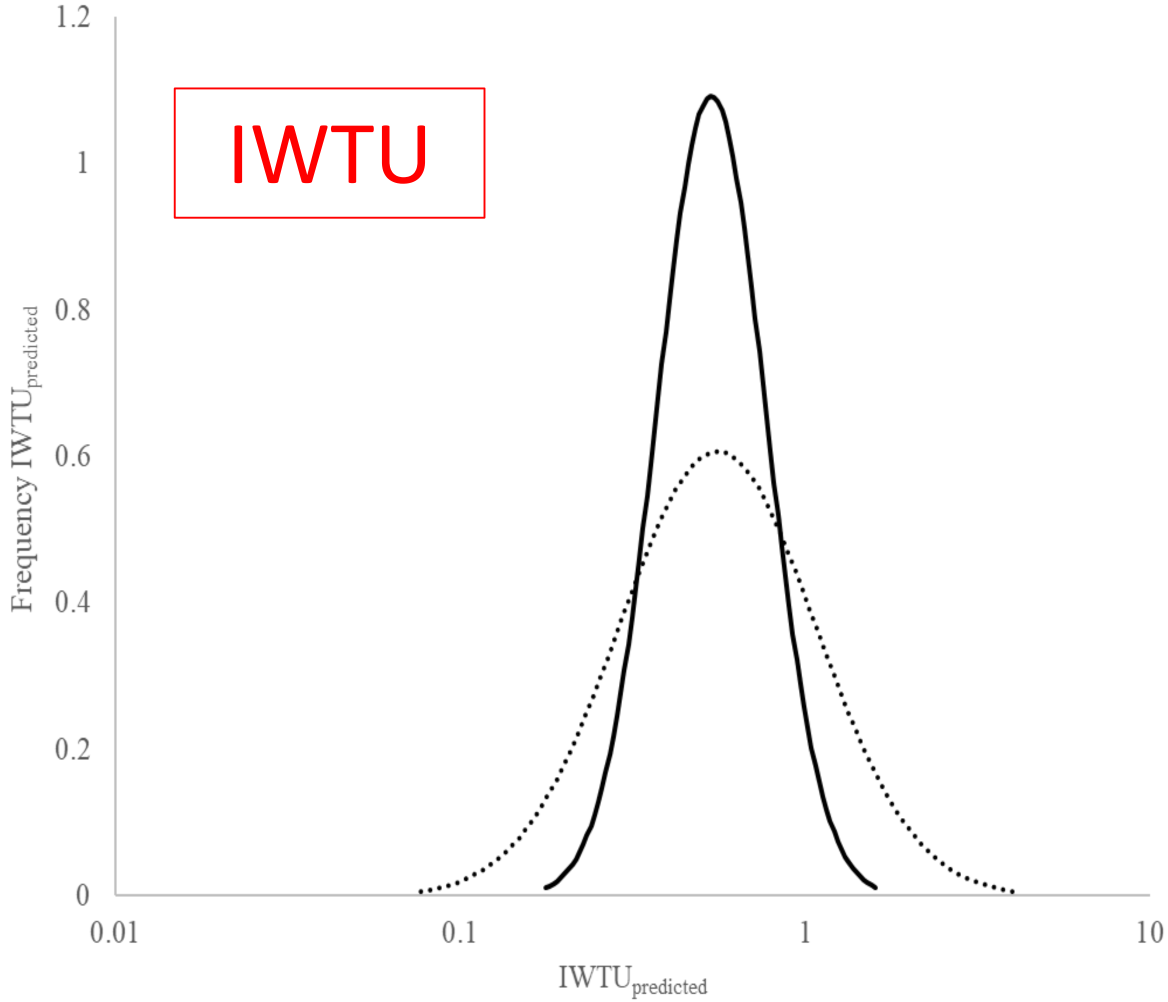
Stochastic Framework



$$BR_i = \frac{\Sigma ESBTU_j}{\Sigma IWTU_j}$$

$\Sigma ESBTU_j$ ← $K_{TOC,default}$

$\Sigma IWTU_j$ ← $K_{TOC,measured}$



For a given ESBTU

Results

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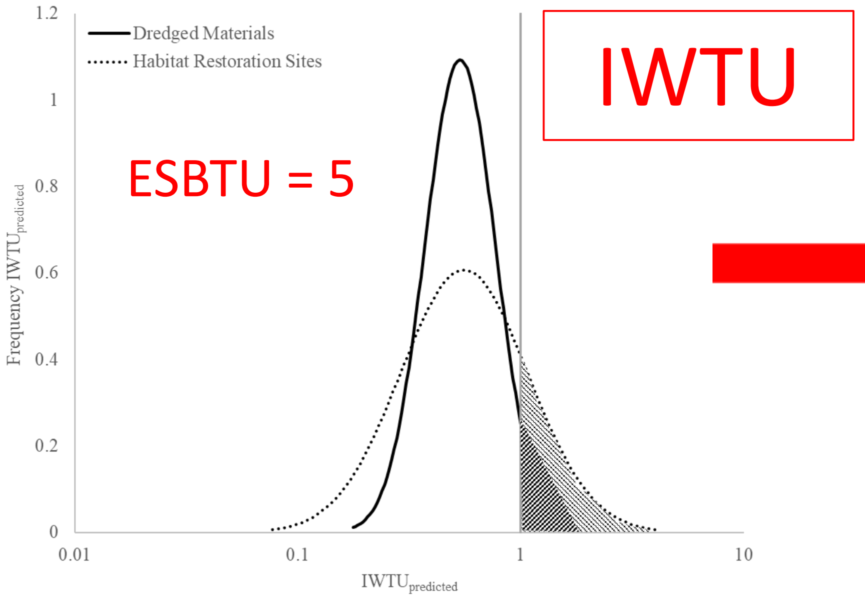
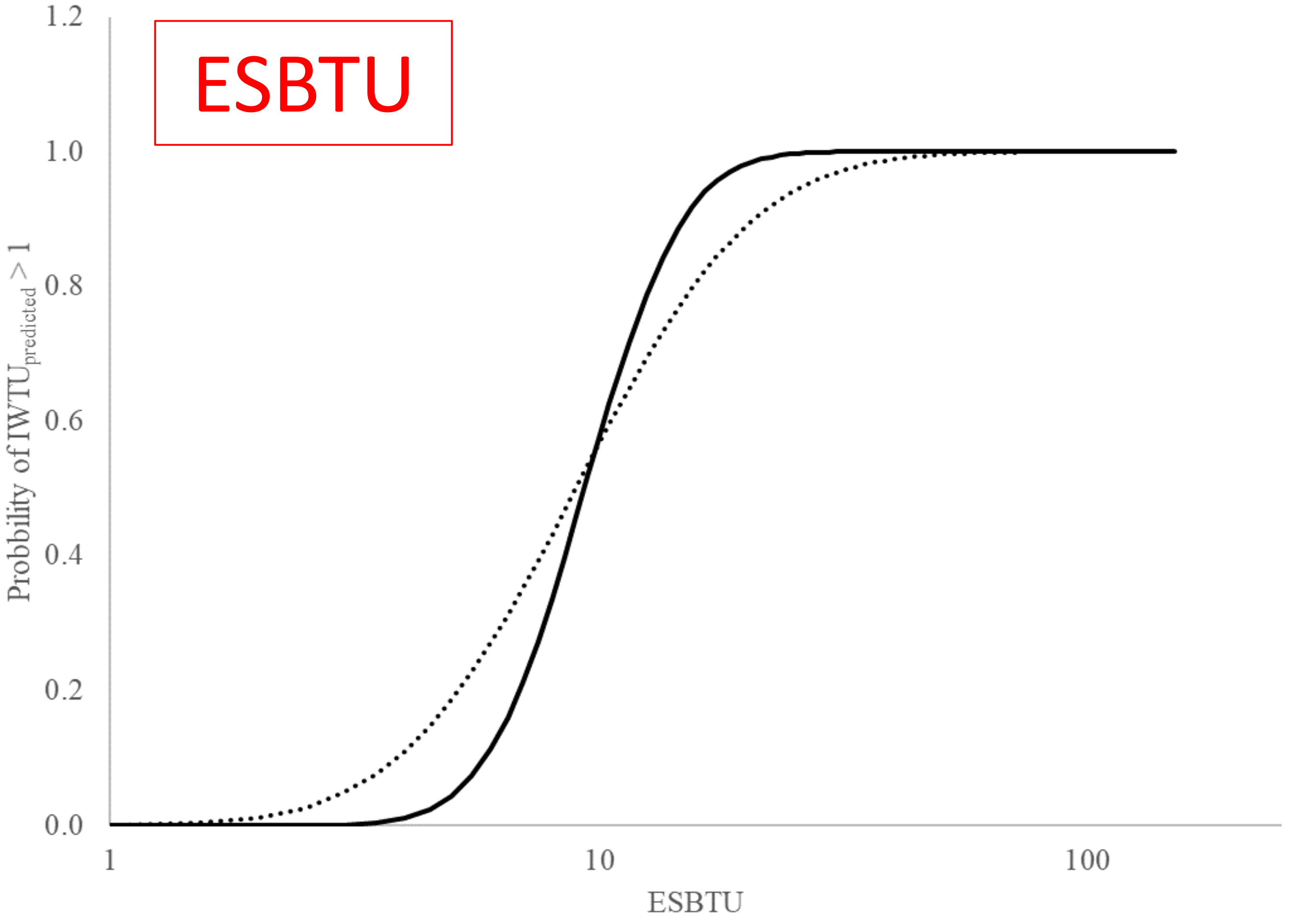
ESBTU ⟶ IWTU



$$IWTU_{predicted}(\mu, \sigma) = \frac{ESBTU_{measured}}{BR(\mu, \sigma)}$$

- Variance in BR has larger effect at lower C_{total}



$$Risk = P\left(\frac{IWTU_{predicted}(\mu, \sigma)}{1.0} > 1\right) = \Phi\left(\frac{\mu_{\ln(IWTU)} - 1.0}{\sigma_{\ln(IWTU)}}\right)$$

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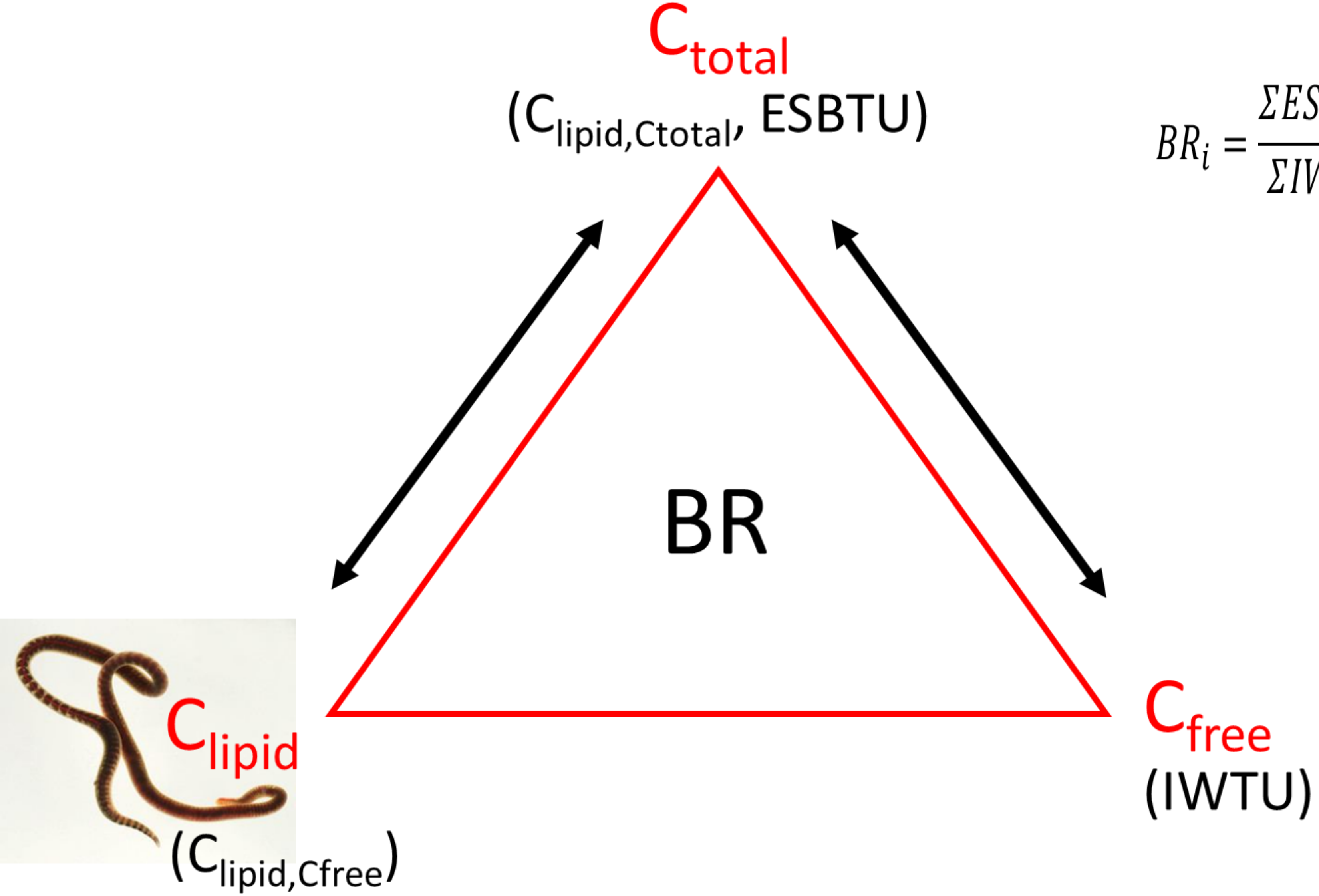
Translating Bioavailability



$$BR_i = \frac{\Sigma ESBTU_j}{\Sigma IWTU_j}$$

$\Sigma ESBTU_j$ ← $K_{TOC,default}$

$\Sigma IWTU_j$ ← $K_{TOC,measured}$

https://alchetron.com/Lumbriculus-variegatus

Conclusions

- **BIOAVAILABILITY RATIO: BR** - provides a quantitative basis for evaluating implications in contaminant partitioning in terms commonly used for risk assessment

- Allows for converting between risk based on C_{free} and cleanup goals based on C_{total}

- Eliminates the need for applying discrete thresholds with conservative assumptions- improves screening-level assessments

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Questions?

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Clean Water Land & Legacy Amendment

Minnesota Pollution Control Agency

US Army Corps of Engineers.

Water Center University of Michigan

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