Predicting the Impacts of Low Levels of Residual Oil: Equilibrium Approach

Joy McGrath

Dominic Di Toro

HydroQual, Inc.

Coastal Response Research Center

University of New Hampshire

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Integrating Physical, Biological and Toxicological Models
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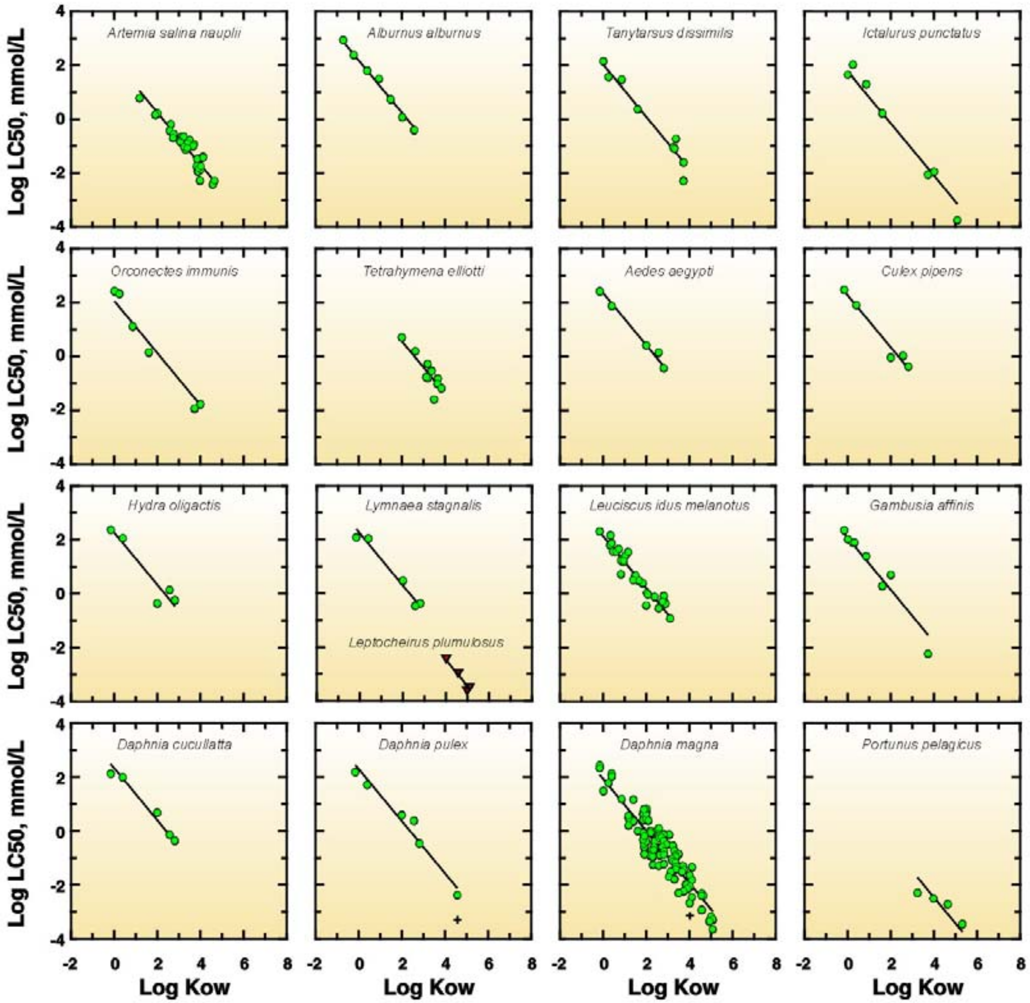
Main Objectives

1. Identify key components of residual oil that contribute to toxicity
2. Establish a universal endpoint that can be applied across different oil sources
3. Derive endpoints for oil-related compounds that are protective of aquatic and benthic species from long-term sub-lethal effects

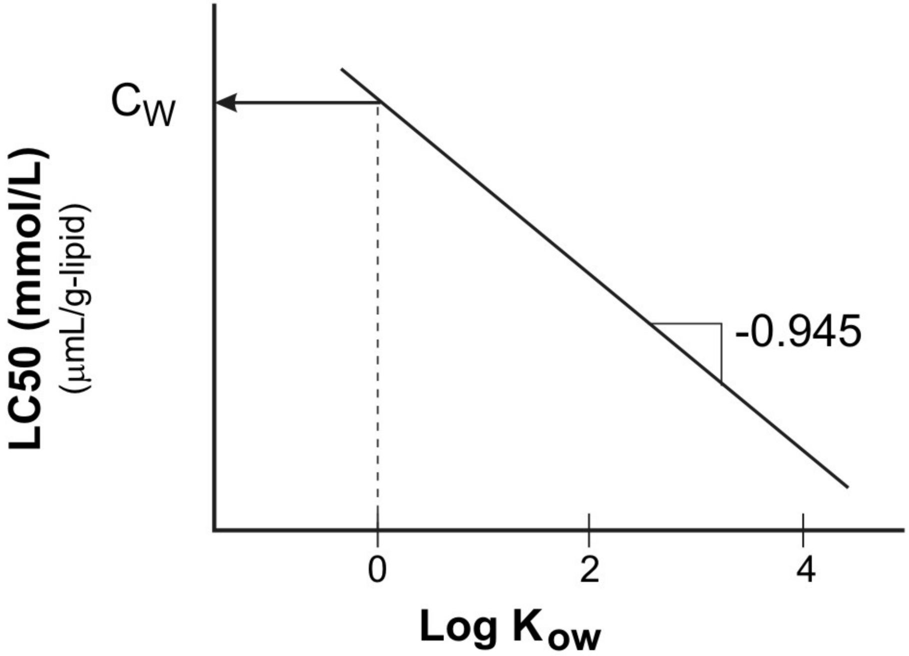
- Toxicity Model is Target Lipid Model (TLM)
- Not Suggesting chronic toxicity of compounds is via narcosis

Acute Toxicity QSARs for Narcotics



(Di Toro et al., ETC, 2000)

Interpretation of Y-Intercept



$K_{OW} = 1$

$C_{OCTANOL} = C_W$

ASSUME: OCTANOL ~ LIPID

$C_{LIPID} = C_W$

$\therefore C_W$ = LC50 BODY BURDEN

(µmol/g-lipid)

Computation of Water-only Effect Concentration

$$\text{Log}\,(C^*_W) = -0.945\,\log(K_{OW}) + \log\,(C^*_L) + cc$$

C^*_L = *Species specific critical target lipid body burden,* $\mu mol/g_{octanol} = \mu mol/g_{lipid}$

cc = Chemical class adjustment, -0.263 for PAHs

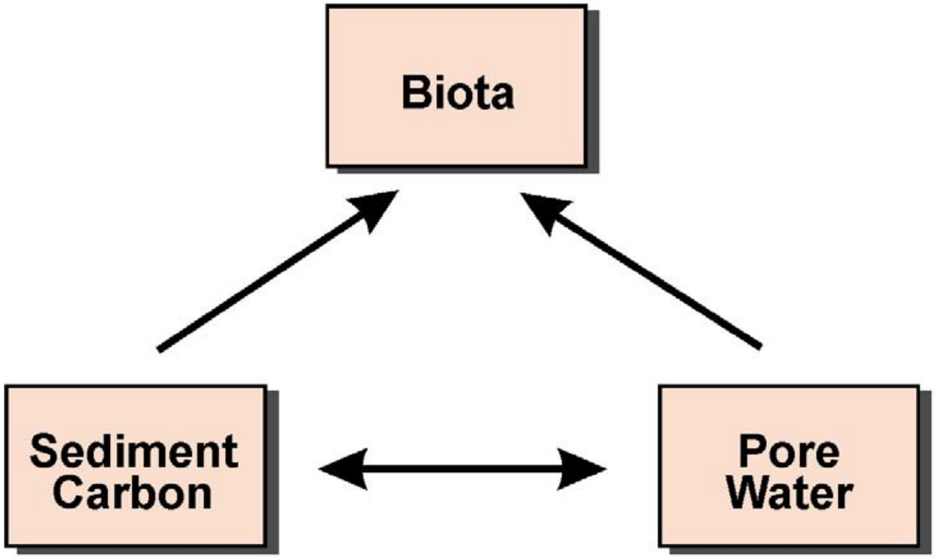
C^*_W = *Acute water-effect concentration, mmol/L*

$$C^*_W\text{, chronic} = \frac{C^*_W\text{, acute}}{ACR}$$

acute

ACR

Sediment-Pore Water Exposure



Equilibrium Partitioning

(Di Toro et al., 1991)

Organic Carbon Normalized Sediment Effect Concentrations

$$C^{*}{}_{s,OC} = K_{OC} \; x \; C^{*}{}_{w}$$

$\mu g/kgOC$ $\quad$ $L/kgOC$ $\quad$ $\mu g/L$

Expression/Normalization of Toxicity

$$TU = \frac{\text{Measured Chemical Concentration in Water, mmol/L}}{C_w^*\text{, mmol/L}}$$

$$TU_{mixture} = \Sigma TU$$

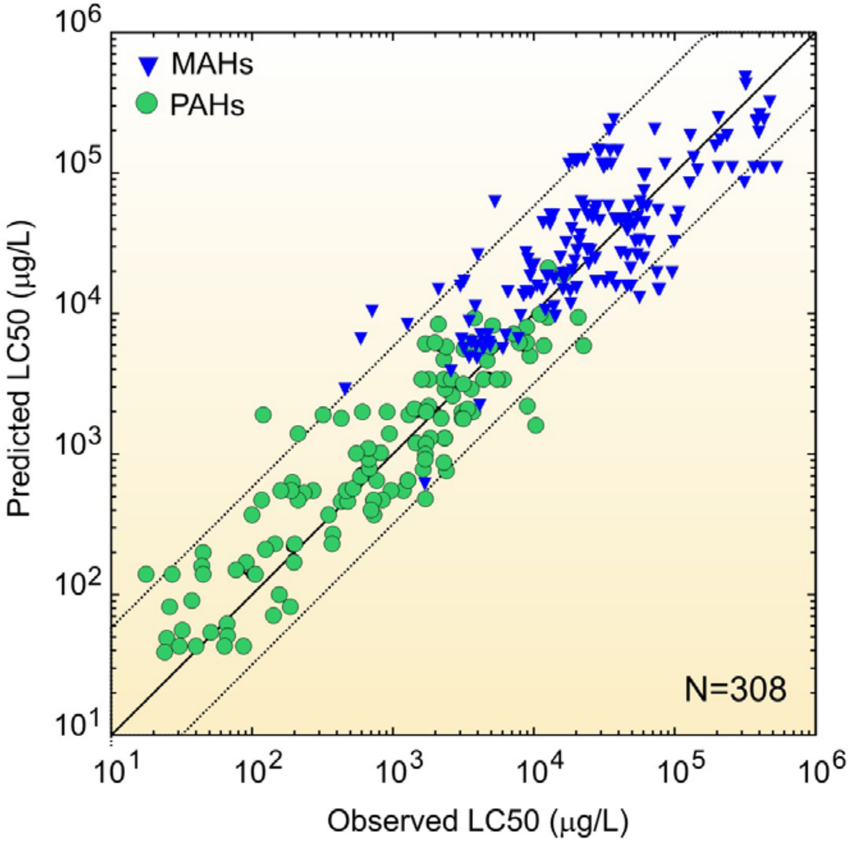
Theoretically $TU \geq 1$	Toxicity predicted
$TU < 0.3$	Toxicity Unlikely
$TU > 2.0$	Toxicity Likely
TU between 0.3 and 2.0	Toxicity Uncertain

Literature Summary

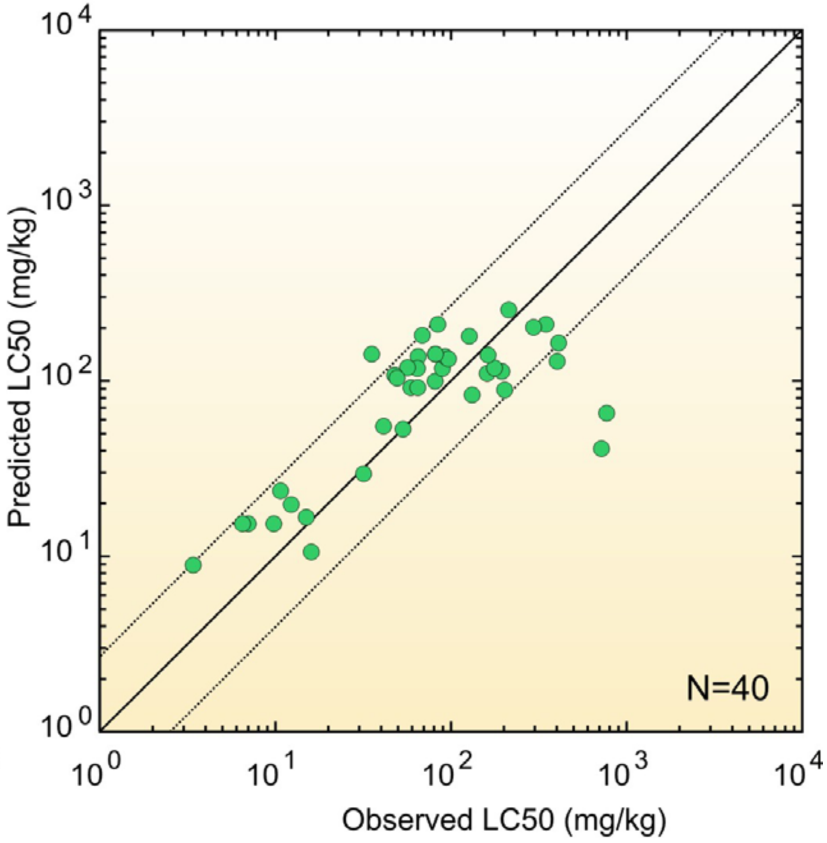
	References Reviewed	References Accepted
Water Column	141	80
Sediment	64	21
TOTAL	205	101

Acute Effects (lethality) – Single Exposures

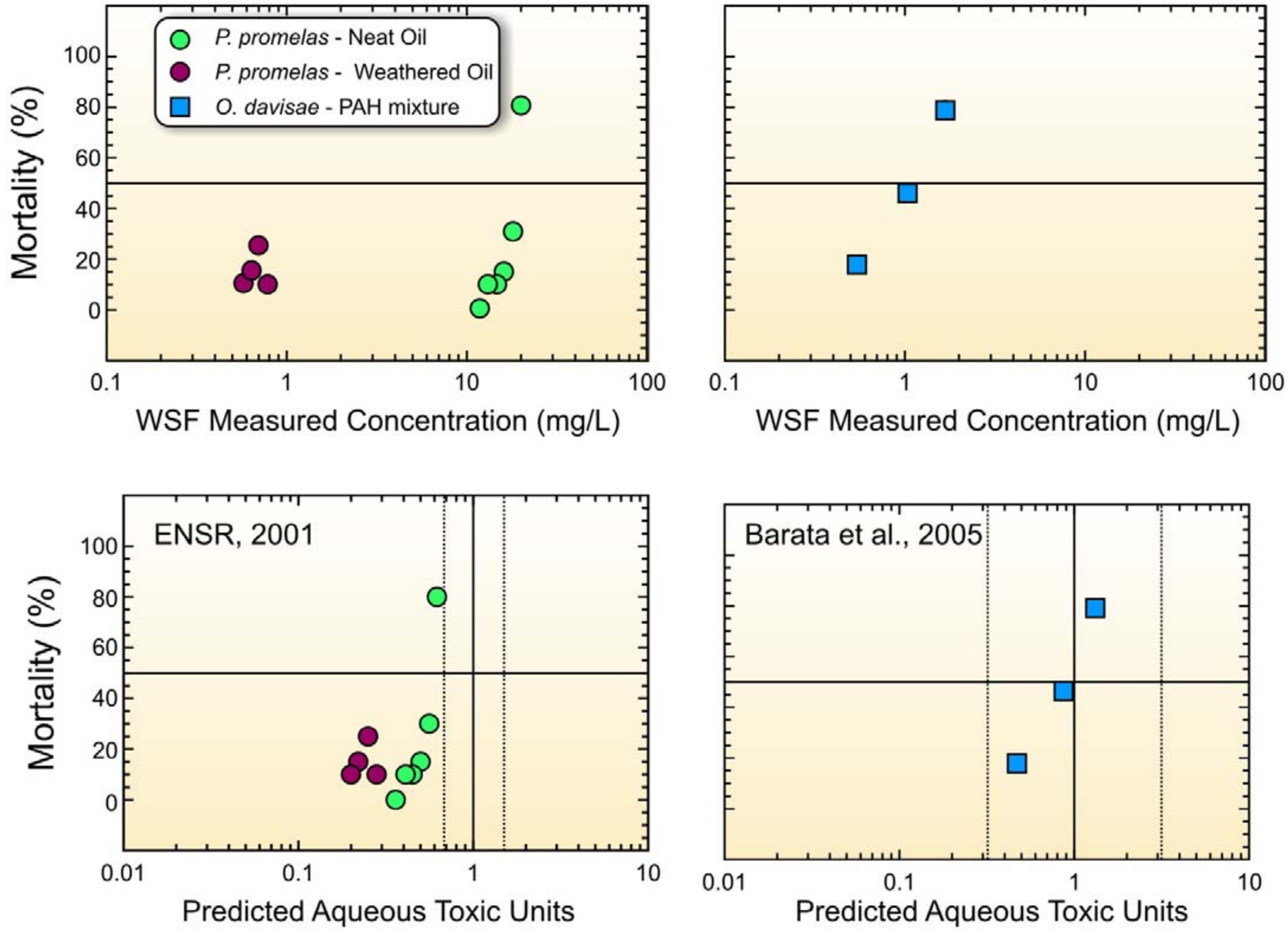
Water Column



Sediment

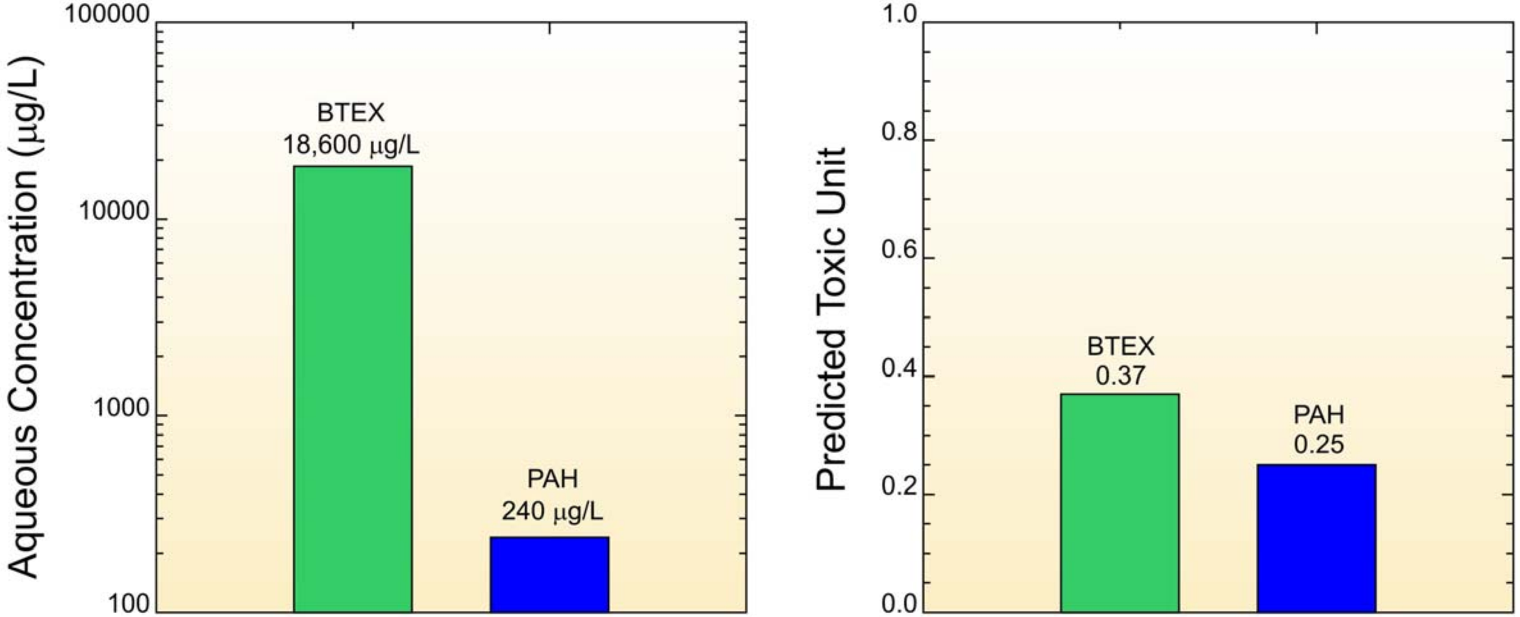


Water Column – Acute Effects
PAH Mixtures



Expression of Toxicity

Neat EVO, 50% Mortality Occurred at ~95% WSF (Total TU = 0.62)



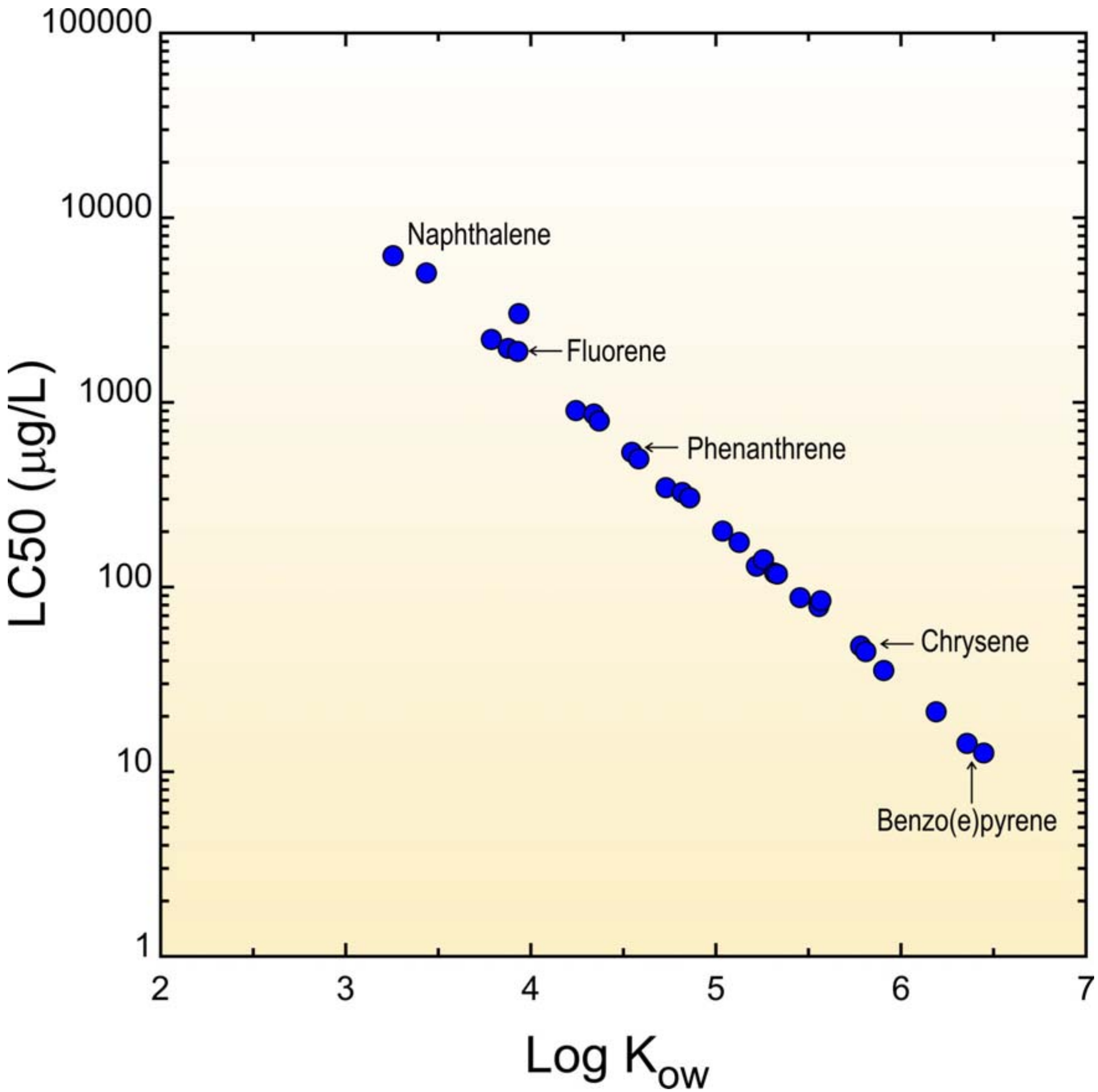
Mass Based: $LC50_{95\%WSF} = LC50_{BTEX} + LC50_{PAH}$

$= 18{,}600 \mu g/L + 240\ \mu g/L = 18{,}840\ \mu g/L$??

TU Based: $TU_{95\%WSF} = TU_{BTEX} + TU_{PAH}$

$= 0.37 + 0.25 = 0.62$

Various PAH LC50s for Fathead Minnows



90% Confidence Limits in Predicted Effect Concentration

$$\log(HC_{95}) \quad + k_Z [\sqrt{\quad}]$$

$$\log(HC_5) = E(m)\log(K_{ow}) + E\{\log(C_L^*)\} - E\{\log(ACR)\} - k_Z\sqrt{V\{m\}\log(K_{OW})^2 + V\{\log(ACR)\} + V\{\log C_L^*\}}$$

Where:

HC_5 = aqueous concentration that protects 95% of organism (mmol/L)

$E\{m\}$ = universal narcosis slope, -0.945

$E\{\log(C_L^*)\}$ = log mean CTLBB mmol/g $_{octanol}$

$E\{\log(ACR)\}$ = log mean acute to chronic ratio.

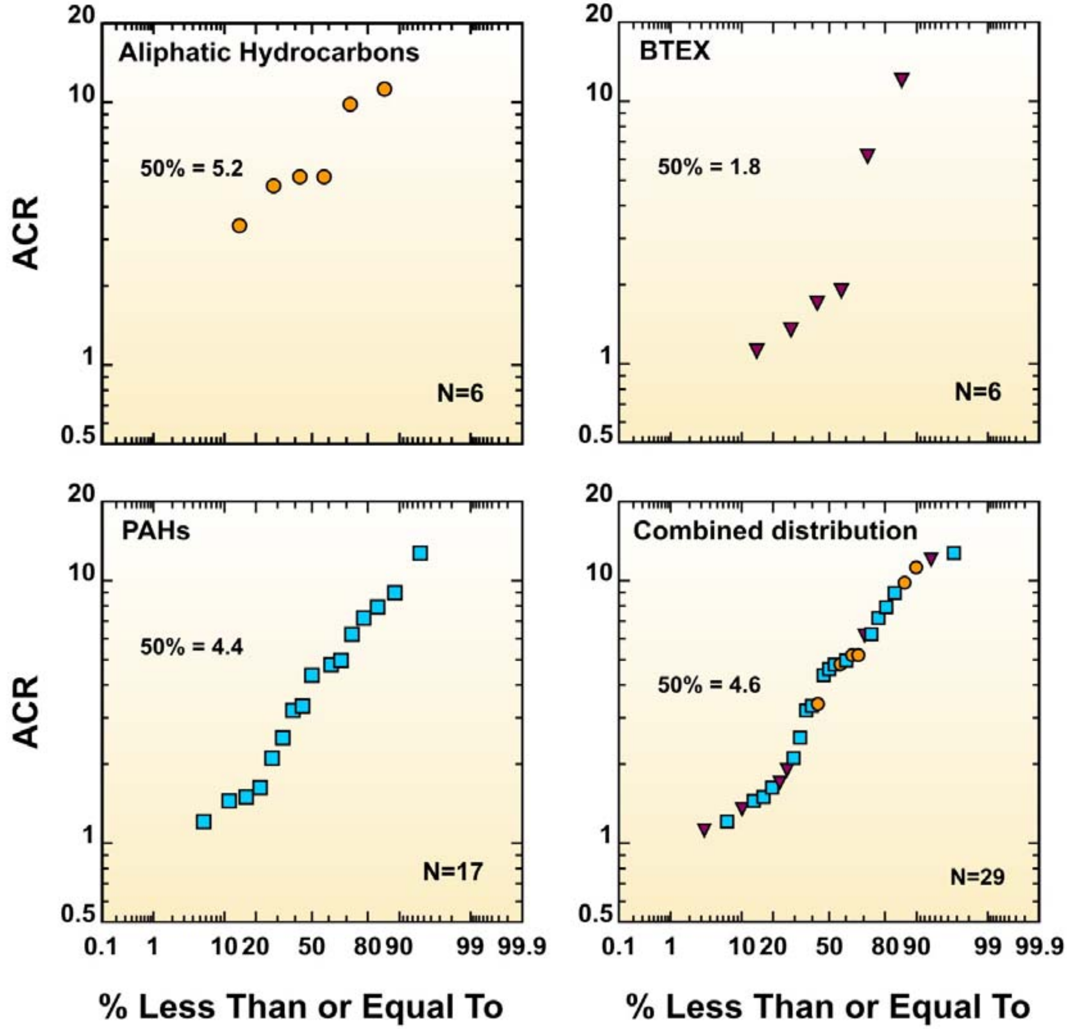
k_Z = 95% confidence sample-size-dependent extrapolation factor,

$V\{m\}\log(K_{OW})$ = variance of universal narcosis slope

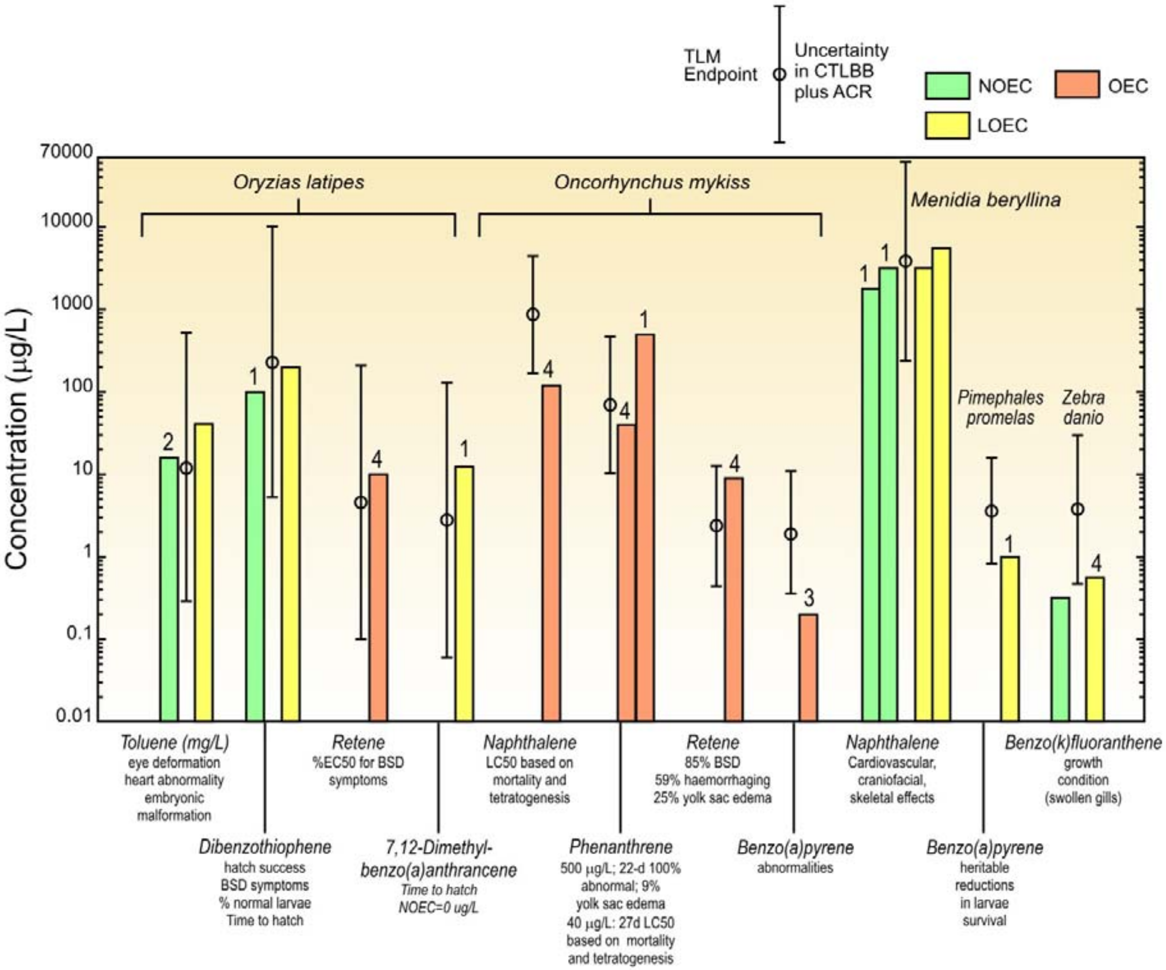
$V\{\log(ACR)\}$ = variance of log (ACR)

$V\{\log C_L^*\}$ = variance of log CTLBB

Chronic Effects (Growth, Reproduction, Mortality) – Single Exposures



Water Column – Other Chronic Sublethal Effects
Single PAH Exposures



Derivation of HC5 Values That Protect 95% of Species

$$\log(HC_5) = E(m)\log(K_{ow}) + E\{\log(C_L^*)\} - E\{\log(ACR)\} - k_Z\sqrt{V\{m\}\log(K_{OW})^2 + V\{\log(ACR)\} + V\{\log C_L^*\}}$$

$E\{\log(C_L^*)\}$ = Geometric mean of all CTLBBs

k_Z = Extrapolation constant based on number of ACRs

$V\{\log C_L^*\}$ = Variance of all CTLBBs

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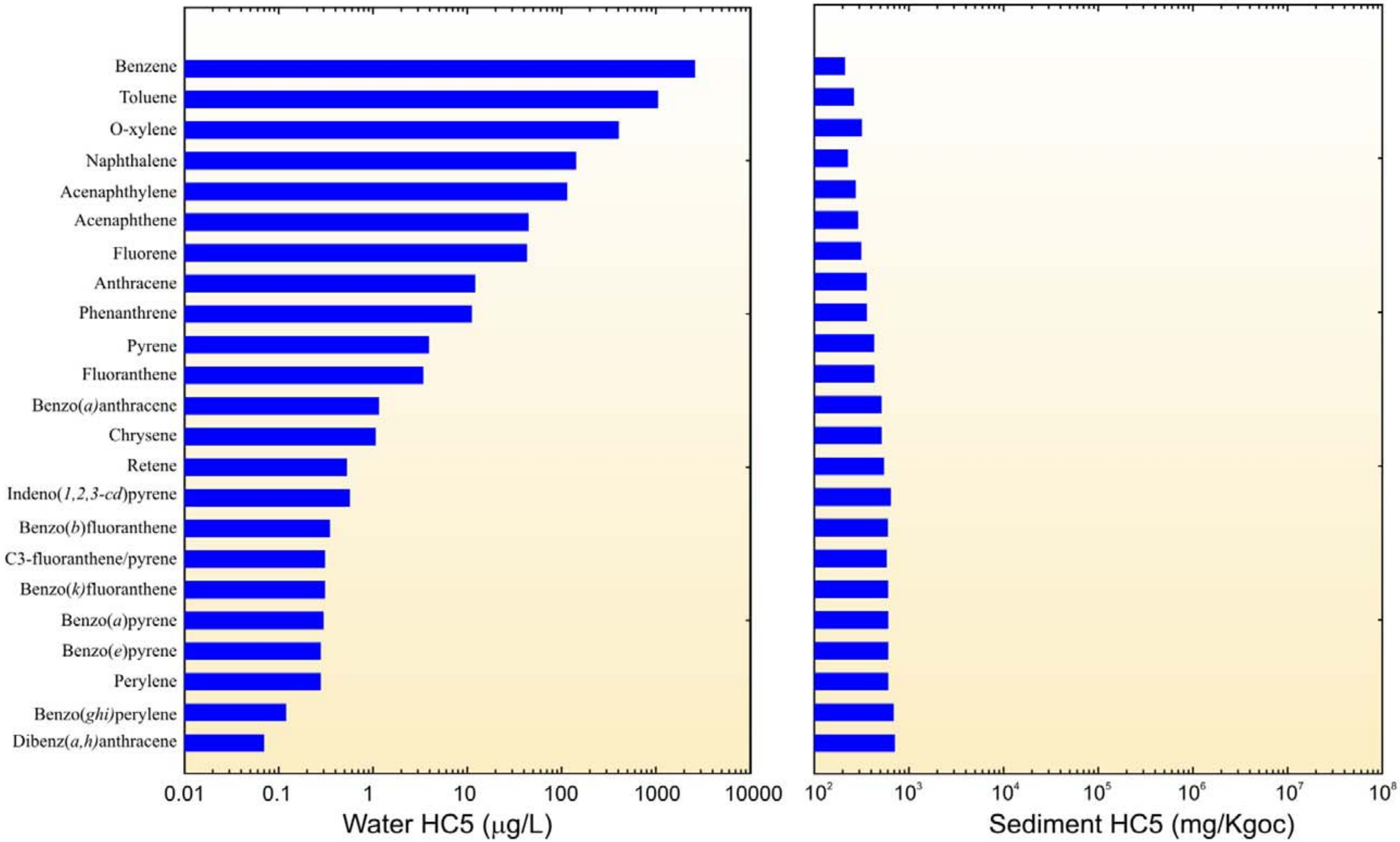
HC5 Values for Water and Sediment



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Comparison of HC5s and NOECs for PAHs