

CONSIDERATION OF TARGET LIPID MODEL FOR USE IN THE DERIVATION OF A HARS-SPECIFIC SCREENING VALUE FOR NON-POLAR ORGANICS.

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CURRENT METHODOLOGY:

The HARS-TEF proposes that critical body residues (CBRs) be utilized to derive an ecological screening value for PAHs and mixtures of non-polar organics. CBRs are defined as the “whole-body concentration of a chemical that is associated with a given adverse biological response” (Rand, 1995). Body residue values can be used to determine the concentration of a contaminant in an organism, at the conclusion of a bioaccumulation test, which may be associated with an adverse effect. Once a screen value is selected, it can potentially be applied to a mixture of PAHs as well as other non-polar organic chemicals including polychlorinated biphenyls (PCBs) and select pesticides. A significant amount of literature is available that supports the CBR approach for PAHs and mixtures of non-polar organic chemicals (McCarty and Mackay, 1993; Broderius et al., 1995; Swartz et al., 1995; Nirmalakhandan et al., 1994; van Wezel and Opperhuizen, 1995; Fisher et al., 1999; Deneer et al., 1988). Overall, the current proposed methodology for deriving a screening value used to evaluate the adverse effects of polynuclear aromatic hydrocarbons (PAHs) and mixtures of non-polar chemicals is “headed in the right direction”. However, the current methodology lacks a scientifically defensible method for selecting a probability based screening value. The current method relies on subjective judgment, limited data, and does not include probability in the process of selecting a screening value. These deficiencies suggest that the current method is not suitable for the derivation of a defensible regulatory screening value.

For the HARS-TEF, Several databases were evaluated including the Jarvinen and Ankley (1999) and the USACE Environmental Residue Effects Database (USACE, 2000) to select the current CBR-based tissue concentration for use as a screening value for non-polar organic chemicals. The lowest effect-concentration (concentration at which changes in survival, growth, reproduction occur) reported in the database was selected following criteria in the HARS-TEF. These criteria included:

- “Residue effects had to be related to impacts on survival, growth, or reproduction...”
- Tissue residues were reported on a whole-body basis
- Data included dose-response information
- Experimental exposures were conducted in the laboratory
- Exposures used post-hatch organisms (i.e., no embryo studies)

In the case of PAHs and non-polar narcotic mixtures, two studies were used to select a value of 0.05 umoles/g tissue (Eertman et al., 1995; Finger et al., 1985). The Eertman et

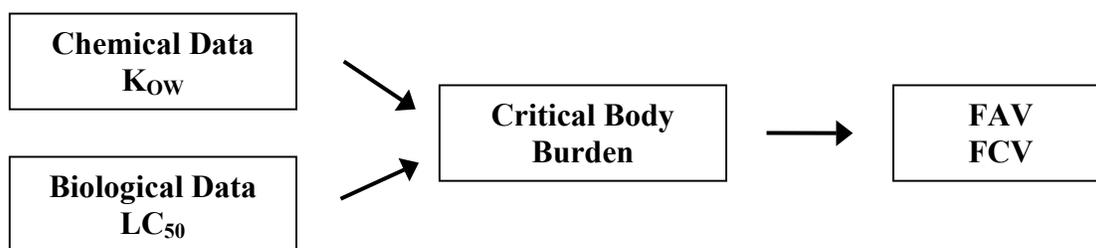
al. study observed a 50% decrease in the clearance rate (TEC_{50}) for the blue mussel (*Mytilus edulus*) corresponding to a fluoranthene tissue concentration of 0.047 umoles/g tissue (dry weight). The second study by Finger et al. observed decreased growth of bluegill fish (*Lepomis macrochirus*) exposed to fluorene for 30 days. The study reports tissue concentrations as “(mg/L) dry weight concentrations”. It is assumed that the authors intended the units to be mg/kg dry weight, however this assumption must be verified through personal communication with the authors prior to its use. Based on this assumption, the lowest effect value calculated from the manuscript for fluorene in bluegill fish is 0.36 umoles/g tissue dry weight. This value does not correspond to the current suggested HARS specific screening value for PAHs and non-polar mixtures (0.05 umoles/g).

Several areas of the HARS-TEF screening value for PAHs and non-polar organic chemicals are deficient and must be corrected prior to implementation. The criteria for selecting studies was not followed in all cases (i.e., the use of *Mytilus* ventilation). In addition, the second study has questionable data as indicated by the improper use of measurement units for tissue concentrations. The selection of the screening value does not include any use of probability and limits itself to the dependence on a single scientific study. It is clear that the current specific method utilized to select a concentration for use as a tissue-based screening value is not scientifically defensible or appropriate for regulatory purposes.

PROPOSED ALTERNATIVE METHODOLOGY:

Guidelines or screening values to assess chemical contamination in soils, sediments, and water are necessary to guide regulatory decisions. The EPA has developed water quality criteria for many contaminants and is in the process of developing guidelines for sediment. In addition, draft guidance for PAH mixtures in sediments has been developed and is currently under review by the Science Advisory Board (EPA, 1999). The approach for assessing PAH mixtures in sediments uses a Final Acute Value, derived from CBR data, to determine concentrations of PAHs in sediments which may result in adverse effects (Di Toro et al., 2000; Di Toro and McGrath, 2000). This approach, which will be outlined in detail below, can be adapted for use in the derivation of a tissue-concentration based effect value that is consistent with the methods used to derive screening values for water and sediment.

The approach outlined by Di Toro et al. (2000) utilizes an accepted relationship between chemical (K_{ow}) and biological (LC_{50}) data to develop critical body burdens (CBBs) following established EPA methods. Numerous studies and species are compiled to develop CBBs. In turn, the CBBs are used to determine probability based Final Acute Value (FAV) and Final Chronic Value (FCV) for non-polar organic chemicals.



Critical body burdens are determined through the use of a relationship between the LC₅₀ values of non-polar organic chemicals and their respective octanol-water partition coefficients (K_{ow}) (Fig. 1). A linear regression using the log transformed LC₅₀ values and log transformed K_{ow} values, previously described by Brezonik (1994) is the linear free energy relationship (LFER). The equation of the line is:

$$\text{Log LC}_{50} = m \log (K_{ow}) + b$$

The slope of the line (m) is the slope of the LFER and is constant for all non-polar organic chemicals regardless of the species tested. From the analysis of many data sets for non-polar organic chemicals with many species, the universal narcosis slope was calculated to be -0.945 ± 0.014 . The y-intercept of the line (b) is the log of the critical target lipid concentration (C_L) for a specific species. C_L is the concentration of chemical in octanol that results in 50% acute mortality.

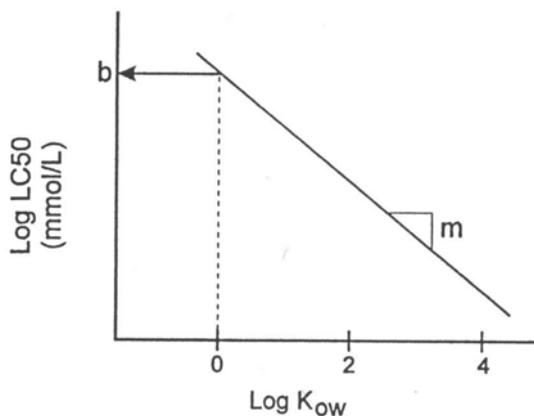


Figure 1. Diagram of LC₅₀ versus K_{ow} relationship. From Di Toro et al., 2000.

The calculation of a CBB for a specific organism and chemical requires a statistically derived chemical class correction factor as a result of the variation in toxic potencies of the chemicals. The chemical class correction factor used for PAHs is 0.546. This chemical class correction factor is used when determining an FAV. The FAV is determined through the compilation of CBBs for different families (Fig. 2). An FAV is the concentration of chemical, based on experimental data, that that will not (based on probability) have an acute narcotic effect on 95% of the organisms. In other words, the value is protective of 95% of all species. These values are calculated following guidance for the derivation of water quality criteria (Stephan et al., 1985).

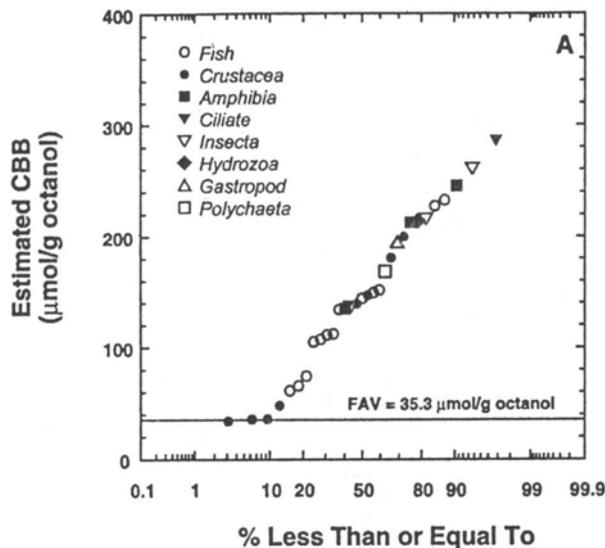


Figure 2. Probability distribution of critical body burdens (C_L) From Di Toro et al., 2000.

The FAV for baseline chemicals is estimated to be 35.3 umol/g octanol (lipid). The FAV for PAHs is 19.3 umoles/g octanol (FAV for baseline chemicals (35.3) multiplied by the chemical class correction factor (0.546)). To determine the FCV, divide the FAV by the acute to chronic ratio (ACR) (Fig. 3). The FCV for PAHs is 3.79 umoles/g octanol. In the case of non-polar organic chemicals, octanol is assumed to have the same or similar properties as lipid (i.e., octanol \cong lipid). Specific FCVs (Table 1) can be derived where lipid data exists for the organisms tested (www.wes.army.mil/el/dots/database.html).

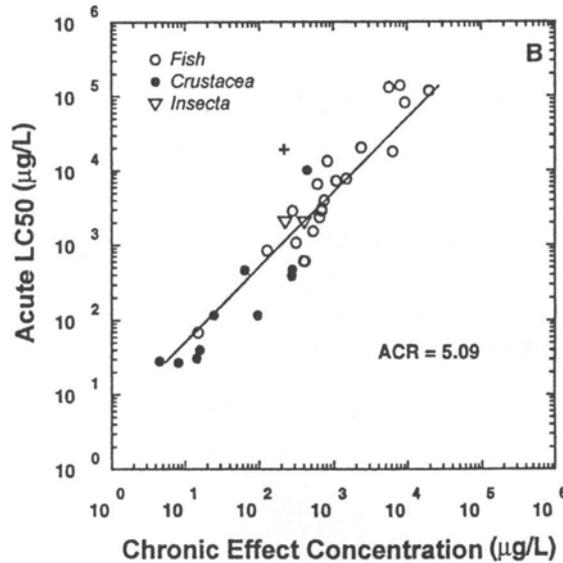


Figure 3. Acute to chronic ratio (ACR) determined from the relationship of acute toxicity versus chronic toxicity concentrations. From Di Toro et al., 2000.

Table 1. FCV values determined for aquatic invertebrates. Values are normalized from lipid-based to whole organism tissue wet weight.

Organism	Percent Lipid	Narcosis FCV umoles/g tissue (wet weight)
<i>Macoma nasuta</i> (clam) ¹	4.83	0.18
<i>Mercenaria sp.</i> (clam) ¹	0.88	0.03
<i>Leptocheirus plumulosus</i> (amphipod) ²	1.78	0.07
<i>Neanthes arenaceodentata</i> (polychaete) ³	2.15	0.08
<i>Nereis virens</i> (polychaete) ¹	7.25	0.27
Average	3.38	0.13

1. USACE BSAF Database: www.wes.army.mil/el/dots/database.html

2. Lotufo, G.R., Farrar, J.D., Duke, B.M. and T.S. Bridges. 2001. DDT toxicity and critical body residue in the amphipod *Leptocheirus plumulosus* in exposures to spiked sediments. *Env. Tox. Chem.* In Press.

3. Lotufo, G.R., Farrar, J.D. and T.S. Bridges. 2000. Effects of exposure source, worm density, and sex on DDT bioaccumulation and toxicity in the marine polychaete *Neanthes arenaceodentata*. *Env. Tox. Chem.* 19:472-484.

CONCLUSION:

The proposed methodology uses existing guidelines currently implemented within the EPA's regulatory framework for assessing water and sediment quality. The total lipid concentration approach includes extensive chemical and biological data in an approach to determine the concentration of a narcotic chemical in an organism's tissue which results in an adverse effect. The proposed approach has the following advantages:

- Utilizes many studies to derive a single value
- Value derived is based on a probability estimate
- Scientifically accepted relationships are used (LFER)
- Established procedures currently implemented for regulatory purposes are used
- The approach is consistent with current regulatory screening concentrations for water and sediment

Overall the proposed approach that integrates chemistry, biology, and established guidance has many advantages over the current HARS-TEF methodology. It is scientifically defensible and will provide a sound basis and guide for regulatory decision making.

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