# APPENDIX B

# DERIVATION OF PAH-SPECIFIC ALGORITHMS

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# DERIVATION OF PAH-SPECIFIC ALGORITHMS

This appendix contains includes derivations of algorithms and parts of algorithms specific to polyaromatic hydrocarbons (PAHs). Section B.1 covers exchanges of PAHs between benthic invertebrates and sediments. Section B.2 includes provides a note about bioaccumulation in fish which can metabolize PAHs. Section B.3 provides a note about dry deposition of PAHs sorbed to airborne particles to plant leaves. The references are provided in Section B.4.

## B.1 EXCHANGES BETWEEN SEDIMENT AND BENTHIC INVERTEBRATES

Uptake of contaminants from water by benthic invertebrates (*e.g.*, mayfly nymphs, amphipods) is primarily based on respiratory processes. Stehly et al. (1990) found that the clearance rate of benzo-a-pyrene (B(a)P) and phenanthrene from water by the mayfly (*i.e.*, mayfly net uptake of the chemical from water) is analogous to the clearance rate (*i.e.*, net uptake rate) of oxygen during mayfly respiration. The uptake of these two PAHs can, therefore, be estimated similarly to the ratio of oxygen clearance to the volume of water passing over respiratory surfaces. With a known or assumed volume of water passing over respiratory membranes with known concentrations of B(a)P and phenanthrene, the extraction efficiency of these PAHs can be calculated. The following concentration algorithms and mass derivatives were adopted from the model of Stehly et al. (1990) for estimating PAH uptake and loss for benthic invertebrates. The equations are based on the clearance rate driven by the volume of water cleared and the bioconcentration factor (BCF). Uptake rates, as measured by a clearance constant (*CLu*), as well as the BCF for 30-, 60-, and 120-day-old mayflies for B(a)P and phenanthrene were provided by Stehly et al. (1990).

$$\frac{dC_{Mayfly}}{dt} = CL_u \times C_W - CL_u \times \frac{C_{Mayfly}}{p_C} \qquad \text{(Eq. B-1)}$$

where:

$C_{Mayfly}$ = concentration of chemical compound in the organism expressed on a wet weight basis (ng[chemical]/g[mayfly wet wt] = mg[chemical]/kg[mayfly wet wt]);

$CL_u$ = clearance constant (equivalent to $k_u$) (mL[water cleared]/g[mayfly wet wt]-hour = L[water cleared]/kg[mayfly wet wt]-(day/24);

$C_W$ = concentration of the chemical in the interstitial water (ng[chemical]/mL[water] = mg[chemical]/L[water]); and

$p_C$ = proportionality constant that relates the concentration of chemical in the organism to the concentration in the exposure water (equivalent to the bioconcentration factor (BCF)) (mg[chemical]/kg[mayfly wet wt] per mg[chemical]/L[water] = L[water]/kg[mayfly wet wt]).

We substitute generic benthic invertebrates (BI) for the mayflies in Stehly et al. (1990). Thus, an estimation of the PAH concentrations in benthic invertebrate populations (*i.e.*, compartments) is as follows:

$$\frac{dN_{BI}}{dt} = \left( n_{BI} \times m_{BI} \times CL_u \times \frac{N_W}{V_W} \times \frac{24}{1000} \right) - \left( CL_u \times \frac{N_{BI}}{p_C} \times 24 \right) \quad \text{(Eq. B-2)}$$

where:

| | | |
|---|---|---|
| $N_{BI}$ | = | mass of chemical in benthic invertebrates (g[chemical]); |
| $n_{BI}$ | = | number of benthic invertebrates (unitless); |
| $m_{BI}$ | = | mass of individual benthic invertebrate organisms (g[BI wet wt]/individual); |
| $N_W$ | = | mass of chemical dissolved in interstitial pore water (g[chemical]); |
| $V_W$ | = | volume of the interstitial pore water (L[water]); |
| 1/1000 | = | units conversion factor (kg/g); and |
| 24 | = | units converstion factor (hr/day). |

Note that:

$$V_{SedW} = V_{Sed} \times \theta \quad \text{(Eq. B-3)}$$

where:

| | | |
|---|---|---|
| $V_{SedW}$ | = | volume of the pore water in the sediment compartment ($m^3$); |
| $V_{Sed}$ | = | volume of the sediment compartment ($m^3$); |
| $\theta$ | = | volume fraction of the sediment compartment that is liquid (*i.e.*, water) (unitless). |

Also note that:

$$Fraction\_Mass\_Dissolved = N_W \times N_{Total} \quad \text{(Eq. B-4)}$$

where:

| | | |
|---|---|---|
| *Fraction_Mass_Dissolved* | = | the fraction of the chemical mass in the sediment compartment that is dissolved in the interstitial water (unitless); |
| $N_W$ | = | chemical inventory dissolved in the interstitial water (g[chemical]); and |
| $N_{Total}$ | = | total chemical inventory in the sediment compartment, both dissolved and associated with sediment particles (g[chemical]). |

As described in Chapter 2, Equation 2-81:

$$f_{ML} = \frac{Fraction\_Mass\_Dissolved}{\theta} \quad \text{(Eq. B-5)}$$

Note that for sediments:

$$\theta = 1 - Volume\_Fraction\_Solid \quad \text{(Eq. B-6)}$$

where:

*Volume_Fraction_Solid* = fraction of sediment compartment that consists of solid sediment particles (unitless),

because the fraction of the sediment compartment that is vapor/gas-phase is assumed to be zero. From those equations, transfer factors can be derived as:

$$T_{SedW \rightarrow BI} = n_{BI} \times m_{BI} \times \frac{CL_u}{V_{SedW}} \times \frac{1}{1000} \times 24 \times f_{ML} \quad \text{(TF B-1)}$$

$$T_{BI \rightarrow SedW} = \frac{CL_u}{p_C} \times 24 \quad \text{(TF B-2)}$$

where:

$T_{SedW \rightarrow BI}$ = transfer factor for PAHs from sediment pore water to benthic invertebrates (/day); and
$T_{BI \rightarrow SedW}$ = transfer factor for PAHs from benthic invertebrates to sediment pore water (/day).

## B.2 BIOACCUMULATION BY FISH

It is possible to use the time-to-equilibrium-based model (Section 6.4.2) for estimating bioaccumulation of nonionic organic chemicals in fish. As described in Section 2.5, some algorithms that represent steady-state equilibrium relationships can be turned into time-dependent ones for use in TRIM.FaTE if an estimate of the time required for the concentration to reach some fraction of the equilibrium value is known. In this case, the concentration of a nonionic organic chemical in a fish compartment at one trophic level (e.g., water-column carnivore, $F_{wcc}$) can be related to the concentration of the chemical in the next lower trophic level (e.g., water-column omnivore $F_{wco}$) by the equilibrium relationship of the form $C_{Fwcc} = K \times C_{Fwco}$. The value of $K$, also known in this context as the bioacumulation factor ($BAF$), and the time $t_\alpha$ required to reach $100\alpha$ percent of the equilibrium must be known or estimated (default $\alpha = 0.95$).

For PAHs, which are readily metabolized by fish, it is appropriate to use a measured wet-weight *BAF* for the PAH chemicals and a measured time to reach $100\times\alpha$ percent of the equilibrium ratio of concentrations in the transfer factor equations TF 6-9 and 6-10. *BAF* values for PAHs can be estimated from $K_{OW}$ values only if the empirical model used (*i.e.*, regression equation) for relating *BAF* to $K_{OW}$ values was derived for fish from a series of PAHs.

## B.3 REFERENCE

Stehly, G. R., Landrum, P. F., Henry, M. G. & Klemm, C. (1990). Toxicokinetics of PAHs in Hexagenia. Environmental Toxicology and Chemistry, 9, 167-174.