

Pesticide tissue residue for single trophic levels:

$$C_B = \frac{k_1 * (m_o * \phi * C_{wto} + m_p * C_{wdp}) + k_D * \sum(P_i C_{Di})}{k_2 + k_E + k_G + k_M}$$

parameters:

k_1 = pesticide uptake rate constant through respiratory area

k_2 = rate constant for elimination of the pesticide through the respiratory area

k_D = pesticide uptake rate constant for uptake through ingestion of food

k_E = rate constant for elimination of the pesticide through excretion of contaminated feces

k_G = organism growth rate constant

k_M = rate constant for pesticide metabolic transformation

m_o = fraction of respiratory ventilation involving overlying water

P_i = fraction of diet containing i (prey item)

ϕ = fraction of the overlying water concentration of the pesticide that is freely dissolved

Calculation of available pesticide fraction in water:

$$\phi = \frac{1}{1 + (X_{POC} * \alpha_{POC} * K_{OW}) + (X_{DOC} * \alpha_{DOC} * K_{OW})}$$

parameters:

X_{POC} = concentration of particulate organic carbon in water

X_{DOC} = concentration of dissolved organic carbon in water

α_{POC} = proportionality constant to describe the similiarity of phase partitioning of POC in relation to octanol

α_{DOC} = proportionality constant to describe the similiarity of phase partitioning of DOC in relation to octanol

Calculation of pesticide concentration in the solid portion of the sediment:

$$C_s = C_{SOC} * OC$$

where:

$$C_{SOC} = C_{WDP} * K_{OC}$$

parameters:

C_{SOC} = normalized (for OC content) pesticide concentration in sediment

C_{WDP} = freely dissolved pesticide concentration in pore water

K_{OC} = organic carbon partition coefficient

OC = percent organic carbon in sediment

Equations associated with the calculation of pesticide clearance through the respiratory system:

For phytoplankton:

$$k_1 = \frac{1}{A + \frac{B}{K_{OW}}}$$

For animals:

$$k_1 = \frac{E_W * G_V}{W_B}$$

where:

$$E_W = \left(1.85 + \frac{155}{K_{OW}}\right)^{-1}$$

$$G_V = 1400 * \left(\frac{W_B^{0.65}}{C_{OX}}\right)$$

parameters:

A = constant related to the resistance to pesticide uptake through the aqueous phase of plant

B = constant related to the resistance to pesticide uptake through the organic phase of plant

C_{ox} = concentration of dissolved oxygen

E_W = pesticide uptake efficiency by gills

G_V = ventilation rate of fish, invertebrates, zooplankton

K_{OW} = octanol water partition coefficient

W_B = wet weight of the organism

Equations associated with the calculation of the respiratory elimination rate constant:

$$k_2 = \frac{k_1}{k_{BW}}$$

where:

$$k_B = V_{LB} * K_{OW} + V_{NB} * \beta * K_{OW} + V_{WB}$$

k_1 = pesticide uptake rate constant for chemical uptake through respiratory area

K_{BW} = organism-water partition coefficient (based on wet weight)

V_{LB} = lipid fraction of organism

V_{NB} = Non Lipid organic matter fraction of animals, Non lipid organic carbon of plants

V_{WB} = water content of the organism

β = proportionality constant expressing the sorption capacity of NLOM or NLOC to that of octanol

Equations involving the calculation of the growth rate constant:

where temperature less than 17.5 degrees C:

$$k_G = 0.0005 * W_B^{-0.2}$$

where temperature is greater than or equal to 17.5 degrees C:

$$k_G = 0.000251 * W_B^{-0.2}$$

W_B = wet weight of the organism

Equations associated with the calculation of the pesticide clearance rate constant through diet:

$$k_D = E_D * \frac{G_D}{W_B}$$

where:

$$E_D = (3 \times 10^{-7} * G_{OW} + 2.0)^{-1}$$

For animals except filter feeders:

$$G_D = 0.022 * W_B^{0.85} * \exp(0.06 * T)$$

For filter feeders:

$$G_D = G_V * C_{SS} * \sigma$$

$$G_V = 1400 * \left(\frac{W_B^{0.65}}{C_{ox}} \right)$$

C_{ox} = concentration of dissolved oxygen

C_{SS} = concentration of suspended solids

E_D = dietary pesticide transfer efficiency

G_D = feeding rate of organism

G_V = ventilation rate of gills

K_{OW} = octanol water partition coefficient

T = temperature

W_B = wet weight of the organism

σ = efficiency of scavenging of particles absorbed from water

Equations associated with the calculation of the fecal elimination rate constant:

$$k_E = G_F * E_D * \frac{K_{GB}}{W_B}$$

where:

$$E_D = (3 \times 10^{-7} * K_{OW} + 2.0)^{-1}$$

$$K_{GB} = \frac{(V_{LG} * K_{OW} + V_{NG} * \beta * K_{OW} + V_{WG})}{V_{LB} * K_{OW} + V_{NB} * \beta * K_{OW} + V_{WB}}$$

$$V_{LG} = \frac{(1 - \varepsilon_L) * V_{LD}}{(1 - \varepsilon_L) * V_{LD} + (1 - \varepsilon_N) * V_{ND} + (1 - \varepsilon_W) * V_{WD}}$$

$$V_{NG} = \frac{(1 - \varepsilon_L) * V_{ND}}{(1 - \varepsilon_L) * V_{LD} + (1 - \varepsilon_N) * V_{ND} + (1 - \varepsilon_W) * V_{WD}}$$

$$V_{WG} = \frac{(1 - \varepsilon_L) * V_{WD}}{(1 - \varepsilon_L) * V_{LD} + (1 - \varepsilon_N) * V_{ND} + (1 - \varepsilon_W) * V_{WD}}$$

$$G_F = [(1 - \varepsilon_L) * V_{LD} + (1 - \varepsilon_N) * V_{ND} + (1 - \varepsilon_w) * V_{WD}] * G_D$$

For animals except filter feeders:

$$G_D = 0.022 * W_B^{0.85} * \exp(0.06 * T)$$

For filter feeders:

$$G_D = G_V * C_{SS} * \sigma$$

$$G_V = 1400 * \left(\frac{W_B^{0.65}}{C_{ox}} \right)$$

Parameters:

C_{ox} = concentration of dissolved oxygen

C_{SS} = concentration of suspended solids

E_D = dietary pesticide transfer efficiency

G_D = feeding rate of organism

G_F = egestion rate of fecal matter

G_V = ventilation rate of gills

k_E = rate constant for elimination of the pesticide through excretion
of contaminated feces

K_{GB} = partition coefficient of the pesticide between the gastrointestinal tract and the organism

K_{OW} = octanol water partition coefficient

T = temperature

V_{LB} = lipid fraction of organism

V_{LD} = overall lipid content of diet

V_{LG} = lipid content in the gut

V_{NB} = NLOM fraction of animals, NLOC of plants

V_{ND} = overall NLOM content of diet

V_{NG} = NLOM content in the gut

V_{WB} = water content of the organism

V_{WD} = overall water content of diet

V_{WG} = water content in the gut

W_B = wet weight of the organism

β = proportionality constant expressing the sorption capacity of NLOM to that of octanol

ε_L = dietary assimilation rate of lipids

ε_N = dietary assimilation rate of NLOM

ε_W = dietary assimilation rate of water

Equations associated with the calculation of the bioconcentration:

where $C_B = C_{BCF}$ when $k_D = k_E = k_G = k_M = 0$:

Calculation of total bioconcentration factor:

$$TotalBCF = \frac{C_{BCF}}{C_{WTO}}$$

where:

Equations associated with the calculation of the lipid normalized bioconcentration factor:

Lipid normalized:

$$BCF = \frac{C_{BCF}/V_{LB}}{C_{WTO} * \phi}$$

Equations associated with the calculation of the bioaccumulation:

$$TotalBAF = \frac{C_B}{C_{WTO}}$$

Equations associated with the calculation of the lipid normalized bioaccumulation factor:

Lipid normalized:

$$BAF = \frac{C_B/V_{LB}}{C_{WTO} * \phi}$$

Equations associated with the calculation of the biomagnification factor:

$$BMF = \frac{C_B/V_{LB}}{\sum [(P_i * C_{Di})/V_{LBi}]}$$

Parameters associated with the calculation of the bioaccumulation, bioconcentration, or biomagnification factors:

C_B = Concentration of pesticide in tissues in a trophic level

C_{WTO} = total chemical concentration in the water column above the sediment

V_{LB} = lipid fraction of organism

P_i = fraction of diet containing prey item i

C_{Di} = concentration of the pesticide in prey item i

V_{LBi} = fraction of lipid in the body of the prey item i

Equations associated with the calculation of dry food ingestion rates:

mammals:

$$FI_{dry} = \frac{(0.0687 * BW^{0.822})}{BW}$$

birds:

$$FI_{dry} = \frac{(0.0582 * BW^{0.651})}{BW}$$

Equations associated with the calculation of wet food ingestion rates:

$$FI_{wet} = \frac{FI_{dry}}{[1 - \sum(P_i * V_{WBi})]}$$

Parameters associated with the calculation of food ingestion rates:

BW = animal body weight

P_i = fraction of diet containing prey item i

V_{WBi} = fraction of water in the body of the prey item i

Equations associated with the calculation of drinking water ingestion rates:

mammals:

$$DW = (0.099 * BW^{0.90})$$

birds:

$$DW = (0.05 * BW^{0.67})$$

Parameters:

BW = Body weight of the animal being assessed

Equations associated with the calculation of EECs:

dose-based:

$$EEC = \sum(P_i * C_{Bi}) * FI_{wet} + \frac{(C_{WTO} * DW)}{BW}$$

dietary-based:

$$EEC = \sum(P_i * C_{Bi})$$

P_i = fraction of diet containing prey item i

C_{Bi} = pesticide tissue residue concentration of each prey item

FI_{wet} = wet food ingestion rate

C_{WTO} = total chemical concentration in the water column above the sediment

DW = drinking water ingestion rate

BW = Body weight of the animal being assessed

Equations associated with the calculation of adjusted dose-based EECs:

mammals:

$$AT = (LD_{50 \text{ or } NOAEL}) * \left(\frac{TW}{AW}\right)^{0.25}$$

birds:

$$AT = LD_{50} * \left(\frac{AW}{TW}\right)^{(x-1)}$$

Parameters:

LD_{50} = endpoint reported by toxicity study

$NOAEL$ = endpoint reported by toxicity study

TW = body weight of tested animal

AW = body weight of assessed mammal

x = Mineau scaling factor