5.7.1.1 Total (Wet and Dry) Particle Phase and Vapor Phase COPC Direct Deposition Load to Water Body (L_{DEP})

As in U.S. EPA (1994r) and NC DEHNR (1997), with the inclusion of the direct deposition of total vapor, we recommend using Equation 5-29 to calculate the load to the water body from the direct deposition of wet and dry particles and vapors onto the surface of the water body (L_{DEP}). The equation is described in detail in Appendix B, Table B-4-8.

Recommended Equation for Calculating:
Total Particle Phase and Vapor Phase Direct Deposition Load to Water Body (L_{DEP})

$$L_{DEP} = Q \cdot [\, F_v \cdot Dytwv + (1 - F_v) \cdot Dytwp \,] \cdot A_W \qquad \text{Equation 5-29}$$

where

L_{DEP} = Total (wet and dry) particle phase and vapor phase COPC direct deposition load to water body (g/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dytwv$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
$Dytwp$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase (s/m^2-yr)
A_W = Water body surface area (m^2)

Appendix A-2 describes how we recommend determining the COPC-specific parameter F_v. Chapter 3 describes generating the modeled air parameters, *Dytwv* and *Dytwp*. Methods for determining the water body surface area, A_w, are described in Chapter 4 and Appendix B.

5.7.1.2 Vapor Phase COPC Diffusion Load to Water Body (L_{dif})

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-30 to calculate L_{dif}. The equation is described in detail in Appendix B, Table B-4-12.

Recommended Equation for Calculating: Vapor Phase COPC Diffusion Load to Water Body (L_{Dif})

$$L_{dif} = \frac{K_v \cdot Q \cdot F_v \cdot Cywv \cdot A_W \cdot 1 \times 10^{-6}}{\dfrac{H}{R \cdot T_{wk}}} \qquad \text{Equation 5-30}$$

where

L_{dif}	=	Vapor phase COPC diffusion load to water body (g/yr)
K_v	=	Overall COPC transfer rate coefficient (m/yr)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
$Cywv$	=	Unitized yearly (water body or watershed) average air concentration from vapor phase (µg-s/g-m^3)
A_W	=	Water body surface area (m^2)
10^{-6}	=	Units conversion factor (g/µg)
H	=	Henry's Law constant (atm-m^3/mol)
R	=	Universal gas constant (atm-m^3/mol-K)
T_{wk}	=	Water body temperature (K)

Calculating the overall COPC transfer rate coefficient (K_v) is described in Section 5.7.4.4, as well as in Appendix B, Table B-4-19. Chapters 2 and 3 explain how we recommend quantifying the COPC emission rate (Q). Appendix A-2 describes how we recommend determining the COPC-specific parameters F_v, H, and R. Chapter 3 describes generating the modeled air parameter, $Cywv$. Methods for determining the water body surface area, A_w, are described in Chapter 4 and Appendix B. Consistent with U.S. EPA (1994r) and U.S. EPA (1998c), we recommend a default water body temperature (T_{wk}) of 298 K (or 25°C).

5.7.1.3 Runoff Load from Impervious Surfaces (L_{RI})

In some watershed soils, a portion of the total (wet and dry) deposition in the watershed will be to impervious surfaces. This deposition may accumulate and be washed off during rain events. As in U.S. EPA (1994r) and NC DEHNR (1997), with the inclusion of total (wet and dry) vapor phase deposition, we recommend using Equation 5-31 to calculate impervious runoff load to a water body (L_{RI}). The equation is also presented in Appendix B, Table B-4-9.

Recommended Equation for Calculating:
Runoff Load from Impervious Surfaces (L_{RI})

$$L_{RI} = Q \cdot [\, F_v \cdot Dytwv + (1.0 - F_v) \cdot Dytwp \,] \cdot A_I \qquad \text{Equation 5-31}$$

where

L_{RI} = Runoff load from impervious surfaces (g/yr)
Q = COPC emission rate (g/s)
F_v = Fraction of COPC air concentration in vapor phase (unitless)
$Dytwv$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from vapor phase (s/m^2-yr)
$Dytwp$ = Unitized yearly (water body or watershed) average total (wet and dry) deposition from particle phase (s/m^2-yr)
A_I = Impervious watershed area receiving COPC deposition (m^2)

Chapters 2 and 3 explain how we recommend quantifying the COPC emission rate (Q). Appendix A-2 describes how we recommend determining the COPC-specific parameter F_v. Chapter 3 describes a method for generating the modeled air parameters, *Dytwv* and *Dytwp*. Impervious watershed area receiving COPC deposition (A_I) is the portion of the total effective watershed area that is impervious to rainfall (such as roofs, driveways, streets, and parking lots) and drains to the water body. Our recommended method for determining A_I is described in Chapter 4 and Appendix B.

5.7.1.4 Runoff Load from Pervious Surfaces (L_R)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-32 to calculate the runoff dissolved COPC load to the water body from pervious soil surfaces in the watershed (L_R). The equation is also presented in Appendix B, Table B-4-10.

Recommended Equation for Calculating:
Runoff Load from Pervious Surfaces (L_R)

$$L_R = RO \cdot (A_L - A_I) \cdot \frac{Cs \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.01$$ Equation 5-32

where

L_R	=	Runoff load from pervious surfaces (g/yr)
RO	=	Average annual surface runoff from pervious areas (cm/yr)
A_L	=	Total watershed area receiving COPC deposition (m^2)
A_I	=	Impervious watershed area receiving COPC deposition (m^2)
Cs	=	Average soil concentration over exposure duration (in watershed soils) (mg COPC/kg soil)
BD	=	Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3
θ_{sw}	=	Soil volumetric water content (ml water/cm^3 soil) = 0.2 ml/cm^3
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
0.01	=	Units conversion factor (kg-cm^2/mg-m^2)

Appendix B describes how we recommend determining the site-specific parameters RO, A_L, A_I, BD, and θ_{sw}. We also address soil bulk density (BD) in Section 5.2.4.2. We also address soil water content (θ_{sw}) in Section 5.2.4.4. Our recommended method for calculating the COPC concentration in watershed soils (Cs) is discussed in Section 5.2.1 and Appendix B, Table B-4-1. Appendix A-2 describes how we recommend calculating the COPC-specific soil/water partition coefficient (Kd_s).

5.7.1.5 Soil Erosion Load (L_E)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-33 to calculate soil erosion load (L_E). The equation is also presented in Appendix B, Table B-4-11.

Recommended Equation for Calculating:
Soil Erosion Load (L_E)

$$L_E = X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001 \qquad \text{Equation 5-33}$$

where

L_E = Soil erosion load (g/yr)
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
ER = Soil enrichment ratio (unitless)
Cs = Average soil concentration over exposure duration (in watershed soils) (mg COPC/kg soil)
BD = Soil bulk density (g soil/cm^3 soil) = 1.5 g/cm^3
$\&_{sw}$ = Soil volumetric water content (ml water/cm^3 soil) = 0.2 ml/cm^3
Kd_s = Soil-water partition coefficient (ml water/g soil)
0.001 = Units conversion factor (k-cm^2/mg-m^2)

Section 5.7.2 describes unit soil loss (X_e). Chapter 4 and Appendix B describe how we recommend determining the site-specific parameters A_L and A_I. We generally recommend calculating the watershed sediment delivery ratio (SD) as described in Section 5.7.3 and in Appendix B, Table B-4-14. COPC concentration in soils (Cs) is described in Section 5.2.1, and Appendix B, Table B-4-1. Soil bulk density (BD) is described in Section 5.2.4.2. Soil water content ($\&_{sw}$) is described in Section 5.2.4.4. Appendix B, Table B-4-11 describes how we recommend determining the COPC-specific soil enrichment ration (ER).

5.7.2 Universal Soil Loss Equation - USLE

As in U.S. EPA (1994g and 1994r), we generally recommend using the universal soil loss equation (USLE), Equation 5-33A, to calculate the unit soil loss (X_e) specific to each watershed. This equation is further described in Appendix B, Table B-4-13. Appendix B also describes how we suggest determining the site- and watershed-specific values for each of the variables associated with Equation 5-33A.

Recommended Equation for Calculating:
Unit Soil Loss (X_e)

$$X_e = RF \cdot K \cdot LS \cdot C \cdot PF \cdot \frac{907.18}{4047} \qquad \text{Equation 5-33A}$$

where

X_e = Unit soil loss (kg/m^2-yr)
RF = USLE rainfall (or erosivity) factor (yr^{-1})
K = USLE erodibility factor (ton/acre)
LS = USLE length-slope factor (unitless)
C = USLE cover management factor (unitless)
PF = USLE supporting practice factor (unitless)
907.18 = Units conversion factor (kg/ton)
4047 = Units conversion factor (m^2/acre)

The USLE RF variable, which represents the influence of precipitation on erosion, is derived from data on the frequency and intensity of storms. This value is typically derived on a storm-by-storm basis, but average annual values have been compiled (U.S. Department of Agriculture 1982). Information on determining site-specific values for variables used in calculating X_e is provided in U.S. Department of Agriculture (U.S. Department of Agriculture 1997) and U.S. EPA guidance (U.S. EPA 1985b). Refer to Appendix B, Table B-4-13 for additional discussion of the USLE.

5.7.3 Sediment Delivery Ratio (*SD*)

We recommend using Equation 5-34 to calculate the sediment delivery ratio (*SD*). The use of this equation is further described in Appendix B, Table B-4-14.

Recommended Equation for Calculating:
Sediment Delivery Ratio *(SD)*

$$SD = a \cdot (A_L)^{-b} \qquad \text{Equation 5-34}$$

where

SD = Sediment delivery ratio (watershed) (unitless)
a = Empirical intercept coefficient (unitless)
b = Empirical slope coefficient (unitless)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)

The sediment delivery ratio (*SD*) for a large land area (i.e. a watershed or part of a watershed) can be calculated, on the basis of the area of the watershed, by using an approach proposed by Vanoni (1975). Accordingly, U.S. EPA (1998c) recommended using Equation 5-34 to calculate the *SD*.

According to Vanoni (1975), sediment delivery ratios vary approximately with the -0.125 power of the drainage area. Therefore, the empirical slope coefficient is assumed to be equal to 0.125. An inspection of the data presented by Vanoni (1975) indicates that the empirical intercept coefficient varies with the size of the watershed, as illustrated in Appendix B, Table B-4-14.

A_L is the total watershed surface area evaluated that is affected by deposition and drains to the body of water (see Chapter 4). In assigning values to the watershed surface area affected by deposition, we generally consider the following relevant:

- the distance from the emission source,
- the location of the area affected by deposition fallout with respect to the point at which drinking water is extracted or fishing occurs
- the watershed hydrology.

5.7.4 Total Water Body COPC Concentration (C_{wtot})

We recommend using Equation 5-35 to calculate the total water body COPC concentration (C_{wtot}). C_{wtot} includes both the water column and the bed sediment. The equation is also presented in Appendix B, Table B-4-15.

Recommended Equation for Calculating: Total Water Body COPC Concentration (C_{wtot})

$$C_{wtot} = \frac{L_T}{Vf_x \cdot f_{wc} + k_{wt} \cdot A_W \cdot (d_{wc} + d_{bs})} \qquad \text{Equation 5-35}$$

where

C_{wtot} = Total water body COPC concentration (including water column and bed sediment) (g COPC/m^3 water body)
L_T = Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
Vf_x = Average volumetric flow rate through water body (m^3/yr)
f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
k_{wt} = Overall total water body COPC dissipation rate constant (yr^{-1})
A_W = Water body surface area (m^2)
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

The total COPC load to the water body (L_T)—including deposition, runoff, and erosion—is described in Section 5.7.1 and Appendix B, Table B-4-7. Average volumetric flow rate through the water body (Vf_x) and water body surface area (A_w) are discussed in Appendix B. Section 5.7.4.1 discusses the fraction of total COPC concentration in the water column (f_{wc}). Section 5.7.4.2 discusses the COPC dissipation rate constant (k_{wt}). Chapter 4 discusses the water body-specific d_{wc}. We discuss the depth of the upper benthic sediment layer (d_{bs}) below.

The depth of the upper benthic layer (d_{bs}), which represents the portion of the bed that is in equilibrium with the water column, cannot be precisely specified; however, U.S. EPA (1998c) recommended values ranging from 0.01 to 0.05. As in U.S. EPA (1994r), we recommend a default value of 0.03, which represents the midpoint of the specified range. Issues related to the remaining parameters are summarized in the following subsections.

Recommended Default Value for: Depth of Upper Benthic Sediment Layer (d_{bs})

0.03 m

5.7.4.1 Fraction of Total Water Body COPC Concentration in the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

We generally recommend using Equation 5-36A to calculate the fraction of total water body COPC concentration in the water column (f_{wc}), and Equation 5-36B to calculate the total water body contaminant concentration in benthic sediment (f_{bs}). The equations are also presented in Appendix B, Table B-4-16.

Recommended Equation for Calculating:
Fraction of Total Water Body COPC Concentration in
the Water Column (f_{wc}) and Benthic Sediment (f_{bs})

$$f_{wc} = \frac{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z}{(1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}) \cdot d_{wc} / d_z + (\theta_{bs} + Kd_{bs} \cdot C_{BS}) \cdot d_{bs} / d_z} \qquad \text{Equation 5-36A}$$

$$f_{bs} = 1 - f_{wc} \qquad \text{Equation 5-36B}$$

where

f_{wc} = Fraction of total water body COPC concentration in the water column (unitless)
f_{bs} = Fraction of total water body COPC concentration in benthic sediment (unitless)
Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS = Total suspended solids concentration (mg/L)
1×10^{-6} = Units conversion factor (kg/mg)
d_z = Total water body depth (m)
θ_{bs} = Bed sediment porosity ($L_{water}/L_{sediment}$)
Kd_{bs} = Bed sediment/sediment pore water partition coefficient (L water/kg bottom sediment)
C_{BS} = Bed sediment concentration (g/cm^3 [equivalent to kg/L])
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

The COPC-specific partition coefficient (Kd_{sw}) describes the partitioning of a contaminant between sorbing material, such as soil, surface water, suspended solids, and bed sediments (see Appendix A-2). Total suspended solids (TSS), total water body depth (d_z), bed sediment porosity (θ_{bs}) and bed sediment concentration (C_{BS}) are addressed below. Bed sediment and sediment pore water partition coefficient

(Kd_{bs}) is discussed in Appendix A-2. Depth of water column (d_{wc}) and depth of upper benthic layer (d_{bs}) are discussed in Section 5.7.4.

U.S. EPA (1998c) and NC DEHNR (1997) recommended using Equations 5-36A and 5-36B to calculate f_{wc} and f_{bs}. NC DEHNR (1997) also recommended adding the depth of the water column to the depth of the upper benthic layer (d_{wc} + d_{bs}) to calculate the total water body depth (d_z).

NC DEHNR (1997) recommended a default total suspended solids (*TSS*) concentration of 10 mg/L, which was adapted from U.S. EPA (1993e). However, due to variability in water body specific values for this variable, we recommend using water body-specific measured *TSS* values representative of long-term average annual values. Average annual values for *TSS* are generally expected to be in the range of 2 to 300 mg/L. Additional information on anticipated *TSS* values is available in U.S. EPA (1998c).

If measured data are not available, or of unacceptable quality, it's possible to calculate a *TSS* value for non-flowing water bodies using Equation 5-36C.

$$TSS = \frac{X_e \cdot (A_L - A_I) \cdot SD \cdot 1x10^3}{Vf_x + D_{ss} \cdot A_W} \qquad \text{Equation 5-36C}$$

where

TSS = Total suspended solids concentration (mg/L)
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving COPC deposition (m^2)
A_I = Impervious watershed area receiving COPC deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
Vf_x = Average volumetric flow rate through water body (value should be 0 for quiescent lakes or ponds) (m^3/yr)
D_{ss} = Suspended solids deposition rate (a default value of 1,825 for quiescent lakes or ponds) (m/yr)
A_W = Water body surface area (m^2)

The default value of 1,825 m/yr provided for D_{ss} is characteristic of Stoke's settling velocity for an intermediate (fine to medium) silt.

Also, it's possible to evaluate the appropriateness of watershed-specific values used in calculating the unit soil loss (X_e), as described in Section 5.7.2 and Appendix B, by comparing the water-body specific measured *TSS* value to the estimated *TSS* value obtained using Equation 5-36C. If the measured and calculated *TSS* values differ significantly, we recommend re-evaluating the parameter values used to calculate X_e. You might also re-evaluate *TSS* and X_e if the calculated *TSS* value is outside of the normal range expected for average annual measured values, as discussed above.

One approach to calculating bed sediment porosity (θ_{bs}) from the bed sediment concentration is by using the following equation (U.S. EPA 1998c):

$$\theta_{bs} = 1 - \frac{C_{BS}}{\rho_s} \qquad \text{Equation 5-37}$$

where

θ_{bs} = Bed sediment porosity ($L_{water}/L_{sediment}$)
ρ_s = Bed sediment density (kg/L)
C_{BS} = Bed sediment concentration (kg/L)

We recommend the following default value for bed sediment porosity (θ_{bs}), adapted from NC DEHNR (1997):

Recommended Value for: **Bed Sediment Porosity (θ_{bs})**
$\theta_{bs} = 0.6$ $L_{water}/L_{sediment}$ assuming $\rho_s = 2.65$ kg/L [bed sediment density] and $C_{BS} = 1.0$ kg/L [bed sediment concentration])

U.S. EPA (1994r) and NC DEHNR (1997) recommended a benthic solids concentration (C_{BS}) ranging from 0.5 to 1.5 kg/L, which was adapted from U.S. EPA (1993e). We recommend the following default value for bed sediment concentration (C_{BS}):

Recommended Default Value for: **Bed Sediment Concentration (C_{BS})**
1.0 kg/L

5.7.4.2 Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-38 to calculate the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial. The equation is also presented in Appendix B, Table B-4-17.

Recommended Equation for Calculating:
Overall Total Water Body COPC Dissipation Rate Constant (k_{wt})

$$k_{wt} = f_{wc} \cdot k_v + f_{bs} \cdot k_b \qquad \text{Equation 5-38}$$

where

k_{wt}	=	Overall total water body dissipation rate constant (yr^{-1})
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
k_v	=	Water column volatilization rate constant (yr^{-1})
f_{bs}	=	Fraction of total water body COPC concentration in benthic sediment (unitless)
k_b	=	Benthic burial rate constant (yr^{-1})

The variables f_{wc} and f_{bs} are discussed in Section 5.7.4.1. The water column volatilization rate constant (k_v) is discussed in Section 5.7.4.3. The benthic burial rate constant (k_b)is discussed in Section 5.7.4.7.

5.7.4.3 Water Column Volatilization Rate Constant (k_v)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-39 to calculate k_v. The equation is also presented in Appendix B, Table B-4-18.

Recommended Equation for Calculating: Water Column Volatilization Rate Constant (k_v)

$$k_v = \frac{K_v}{d_z \cdot (1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6})} \qquad \text{Equation 5-39}$$

where

k_v = Water column volatilization rate constant (yr^{-1})
K_v = Overall COPC transfer rate coefficient (m/yr)
d_z = Total water body depth (m)
Kd_{sw} = Suspended sediments/surface water partition coefficient (L water/kg suspended sediments)
TSS = Total suspended solids concentration (mg/L)
1×10^{-6} = Units conversion factor (kg/mg)

The overall transfer rate coefficient (K_v) is discussed in Section 5.7.4.4. Total water body depth (d_z), suspended sediment and surface water partition coefficient (Kd_{sw}), and total suspended solids concentration (TSS), are described in Section 5.7.4.1. Kd_{sw} is also discussed in Appendix A-2.

5.7.4.4 Overall COPC Transfer Rate Coefficient (K_v)

Volatile organic chemicals can move between the water column and the overlying air. The overall transfer rate K_v, or conductivity, is determined by a two-layer resistance model that assumes that two “stagnant films” are bounded on either side by well-mixed compartments. Concentration differences serve as the driving force for the water layer diffusion. Pressure differences drive the diffusion for the air layer. From balance considerations, the same mass must pass through both films; the two resistances thereby combine in series, so that the conductivity is the reciprocal of the total resistance.

As in U.S. EPA (1993f; 1993e; 1998c), and NC DEHNR (1997), we recommend using Equation 5-40 to calculate K_v. The equation is also presented in Appendix B, Table B-4-19.

Recommended Equation for Calculating:
Overall COPC Transfer Rate Coefficient (K_v)

$$K_v = \left(K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{wk}} \right)^{-1} \right)^{-1} \cdot \theta^{T_{wk} - 293} \qquad \text{Equation 5-40}$$

where

K_v = Overall COPC transfer rate coefficient (m/yr)
K_L = Liquid phase transfer coefficient (m/yr)
K_G = Gas phase transfer coefficient (m/yr)
H = Henry's Law constant (atm-m^3/mol)
R = Universal gas constant (atm-m^3/mol-K)
T_{wk} = Water body temperature (K)
θ = Temperature correction factor (unitless)

The liquid and gas phase transfer coefficients, K_L and K_G, respectively, vary with the type of water body. We discuss the liquid phase transfer coefficient (K_L) in Section 5.7.4.5, and the gas phase transfer coefficient (K_G) in Section 5.7.4.6.

Henry's Law constants generally increase with increasing vapor pressure of a COPC and generally decrease with increasing solubility of a COPC. Henry's Law constants are COPC-specific and we offer recommended default values in the HHRAP companion database. The universal ideal gas constant, R, is 8.205×10^{-5} atm-m^3/mol-K, at 20°C. The temperature correction factor (θ), which is equal to 1.026, adjusts for the actual water temperature. Equation 5-40 assumes that volatilization occurs much less readily in lakes and reservoirs than in moving water bodies.

The value of the conductivity K_v depends on the intensity of turbulence in the water body and the overlying atmosphere. As Henry's Law constant increases, the conductivity tends to be increasingly influenced by the intensity of turbulence in water. Conversely, as Henry's Law constant decreases, the value of the conductivity tends to be increasingly influenced by the intensity of atmospheric turbulence.

5.7.4.5 Liquid Phase Transfer Coefficient (K_L)

We generally recommend using Equations 5-41A and 5-41B to calculate liquid phase transfer coefficient. (K_L). The use of these equations is further described in Appendix B, Table B-4-20.

Recommended Equation for Calculating: Liquid Phase Transfer Coefficient (K_L)

For flowing streams or rivers:

$$K_L = \sqrt{\frac{(1 \times 10^{-4}) \cdot D_w \cdot u}{d_z}} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-41A}$$

For quiescent lakes or ponds:

$$K_L = (C_d^{0.5} \cdot W) \cdot \left(\frac{\rho_a}{\rho_w}\right)^{0.5} \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_w}{\rho_w \cdot D_w}\right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-41B}$$

where

K_L = Liquid phase transfer coefficient (m/yr)
D_w = Diffusivity of COPC in water (cm^2/s)
u = Current velocity (m/s)
1×10^{-4} = Units conversion factor (m^2/cm^2)
d_z = Total water body depth (m)
C_d = Drag coefficient (unitless)
W = Average annual wind speed (m/s)
ρ_a = Density of air (g/cm^3)
ρ_w = Density of water (g/cm^3)
k = von Karman's constant (unitless)
λ_z = Dimensionless viscous sublayer thickness (unitless)
μ_w = Viscosity of water corresponding to water temperature (g/cm-s)
3.1536×10^7 = Units conversion factor (s/yr)

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using the following default values:

- a diffusivity of chemical in water ranging (D_w) from 1.0×10^{-5} to 8.5×10^{-2} cm^2/s,
- a drag coefficient (C_d) of 0.0011 which was adapted from U.S. EPA (1998c),
- a density of air (ρ_a) of 0.0012 g/cm^3 at standard conditions (temperature = 20°C or 293 K, pressure = 1 atm or 760 millimeters of mercury) (Weast 1986),
- a density of water (ρ_w) of 1 g/cm^3 (Weast 1986),
- a von Karman's constant (k) of 0.4,
- a dimensionless viscous sublayer thickness (λ_z) of 4,
- a viscosity of water (μ_w) of a 0.0169 g/cm-s corresponding to water temperature (Weast 1986).

The values above are further discussed in Appendix A-2. Chapter 4 discusses the current velocity (u). Chapter 3 describes methods for determining the average annual wind speed (W). Section 5.7.4.1 discusses the total water body depth (d_z) for liquid phase transfer coefficients.

For a flowing stream or river, the transfer coefficients are controlled by flow-induced turbulence. For these systems, we recommend calculating K_L using Equation 5-41A, which is the O'Connor and Dobbins (1958) formula, as presented in U.S. EPA (1998c).

For a stagnant system (quiescent lake or pond), the transfer coefficient is controlled by wind-induced turbulence. For quiescent lakes or ponds, we recommend calculating K_L using Equation 5-41B (O'Connor 1983; U.S. EPA 1998c).

5.7.4.6 Gas Phase Transfer Coefficient (K_G)

We generally recommend using Equations 5-42A and 5-42B to calculate gas phase transfer coefficient (K_G). The equation is also discussed in Appendix B, Table B-4-21.

Recommended Equation for Calculating:
Gas Phase Transfer Coefficient (K_G)

For flowing streams or rivers:

$$K_G = 36500 \text{ m/yr} \qquad \text{Equation 5-42A}$$

For quiescent lakes or ponds:

$$K_G = (C_d^{0.5} \cdot W) \cdot \frac{k^{0.33}}{\lambda_z} \cdot \left(\frac{\mu_a}{\rho_a \cdot D_a}\right)^{-0.67} \cdot 3.1536 \times 10^7 \qquad \text{Equation 5-42B}$$

where

K_G = Gas phase transfer coefficient (m/yr)
C_d = Drag coefficient (unitless)
W = Average annual wind speed (m/s)
k = von Karman's constant (unitless)
λ_z = Dimensionless viscous sublayer thickness (unitless)
μ_a = Viscosity of air corresponding to air temperature (g/cm-s)
ρ_a = Density of air corresponding to water temperature (g/cm^3)
D_a = Diffusivity of COPC in air (cm^2/s)
3.1536×10^7 = Units conversion factor (s/yr)

The following parameters, including default values, are discussed in Section 5.7.4.5, and in Appendix A-2: C_d, k, λ_z, and ρ_a. Chapter 3 describes methods for determining the average annual wind speed (W). As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using a value of 1.81 x 10^{-4} g/cm-s for the viscosity of air corresponding to air temperature (μ_a). Appendix A-2 discusses the COPC-specific parameter D_a.

U.S. EPA (1998c) indicated that the rate of transfer of a COPC from the gas phase for a flowing stream or river is assumed to be constant, in accordance with O'Connor and Dobbins (1958) (Equation 5-42A).

For a stagnant system (quiescent lake or pond), the transfer coefficients are controlled by wind-induced turbulence. For quiescent lakes or ponds, we recommend calculating the gas phase transfer coefficient using the equation presented in O'Connor (1983) (Equation 5-42B).

5.7.4.7 Benthic Burial Rate Constant (k_b)

We generally recommend using Equation 5-43 to calculate benthic burial rate (k_b). The equation is also discussed in Appendix B, Table B-4-22.

Recommended Equation for Calculating:
Benthic Burial Rate Constant (k_b)

$$k_b = \left(\frac{X_e \cdot A_L \cdot SD \cdot 1\times10^3 - Vf_x \cdot TSS}{A_W \cdot TSS} \right) \cdot \left(\frac{TSS \cdot 1\times10^{-6}}{C_{BS} \cdot d_{bs}} \right) \qquad \text{Equation 5-43}$$

where

k_b = Benthic burial rate constant (yr^{-1})
X_e = Unit soil loss (kg/m^2-yr)
A_L = Total watershed area (evaluated) receiving deposition (m^2)
SD = Sediment delivery ratio (watershed) (unitless)
Vf_x = Average volumetric flow rate through water body (m^3/yr)
TSS = Total suspended solids concentration (mg/L)
A_W = Water body surface area (m^2)
C_{BS} = Bed sediment concentration (g/cm^3)
d_{bs} = Depth of upper benthic sediment layer (m)
1 x 10^{-6} = Units conversion factor (kg/mg)
1 x 10^3 = Units conversion factor (g/kg)

Section 5.7.2 discusses the unit soil loss (X_e). Section 5.7.3 discusses watershed area evaluated receiving COPC deposition (A_L) and sediment delivery ratio (SD). Average volumetric flow rate through the water body (Vf_x) and water body surface area (A_w) are discussed in Appendix B. A_w is also discussed in Appendix A-2. Section 5.7.4.1 discusses total suspended solids concentration (TSS) and bed sediment concentration (C_{BS}). Section 5.7.4 discusses the depth of the upper benthic sediment layer (d_{bs}).

It's possible to express the benthic burial rate constant (k_b), which is calculated in Equation 5-43, in terms of the rate of burial (Wb):

$$Wb = k_b \cdot d_{bs} \qquad \text{Equation 5-44}$$

where

Wb = Rate of burial (m/yr)
k_b = Benthic burial rate constant (yr^{-1})
d_{bs} = Depth of upper benthic sediment layer (m)

According to U.S. EPA (1994r) and NC DEHNR (1997), COPC loss from the water column resulting from burial in benthic sediment can be calculated using Equation 5-43.

We expect k_b values to range from 0 to 1.0: Low k_b values for water bodies with limited or no sedimentation (rivers and fast flowing streams), and k_b values closer to 1.0 for water bodies characteristic of higher sedimentation (lakes). This range of values is based on the relation between the benthic burial rate and rate of burial expressed in Equation 5-44; with the depth of upper benthic sediment layer held constant. If you calculate a negative k_b value (water bodies with high average annual volumetric flow rates in comparison to watershed area evaluated), we recommend using a k_b value of 0 in calculating the total water body COPC concentration (C_{wtot}) in Equation 5-35. If the calculated k_b value exceeds 1.0, we recommend re-evaluating the parameter values used in calculating X_e. Our experience has shown that the value calculated for X_e is the most likely reason for estimating a large and potentially unrealistic benthic burial rate. Information about determining site-specific values and variables for calculating Xe are in the references cited in Section 5.7.2.

5.7.4.8 Total COPC Concentration in Water Column (C_{wctot})

As in U.S. EPA (1994r) and NC DEHNR (1997), we generally recommend using Equation 5-45 to calculate total COPC concentration in water column (C_{wctot}). The equation is also discussed in Appendix B, Table B-4-23.

Recommended Equation for Calculating:
Total COPC Concentration in Water Column (C_{wctot})

$$C_{wctot} = f_{wc} \cdot C_{wtot} \cdot \frac{d_{wc} + d_{bs}}{d_{wc}}$$ Equation 5-45

where

C_{wctot}	=	Total COPC concentration in water column (mg COPC/L water column)
f_{wc}	=	Fraction of total water body COPC concentration in the water column (unitless)
C_{wtot}	=	Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
d_{wc}	=	Depth of water column (m)
d_{bs}	=	Depth of upper benthic sediment layer (m)

We discussed the fraction of total water body COPC concentration in the water column (f_{wc}) in Section 5.7.4.1. We discussed the total COPC Concentration in the water column (C_{wctot}), as well as depth of the water column (d_{wc}) and benthic sediment layer (d_{bs}) in Section 5.7.4.

5.7.4.9 Dissolved Phase Water Concentration (C_{dw})

We recommend using Equation 5-46 to calculate the concentration of COPC dissolved in the water column (C_{dw}). The equation is discussed in detail in Appendix B, Table B-4-24.

Recommended Equation for Calculating:
Dissolved Phase Water Concentration (C_{dw})

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \cdot TSS \cdot 1 \times 10^{-6}}$$ Equation 5-46

where

C_{dw}	=	Dissolved phase water concentration (mg COPC/L water)
C_{wctot}	=	Total COPC concentration in water column (mg COPC/L water column)
Kd_{sw}	=	Suspended sediments/surface water partition coefficient (L water/kg suspended sediment)
TSS	=	Total suspended solids concentration (mg/L)
1×10^{-6}	=	Units conversion factor (kg/mg)

We discussed C_{wctot} in Section 5.7.4.8. We discussed Kd_{sw} and TSS in Section 5.7.4.1.

Using Equation 5-46 to calculate the concentration of COPC dissolved in the water column is consistent with recommendations in U.S. EPA (1994r) and NC DEHNR (1997).

5.7.4.10 COPC Concentration Sorbed to Bed Sediment (C_{sb})

We recommend using Equation 5-47 to calculate COPC concentration sorbed to bed sediment (C_{sb}). The equation is also presented in Appendix B, Table B-4-25.

Recommended Equation for Calculating:
COPC Concentration Sorbed to Bed Sediment (C_{sb})

$$C_{sb} = f_{bs} \cdot C_{wtot} \cdot \left(\frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot C_{BS}} \right) \cdot \left(\frac{d_{wc} + d_{bs}}{d_{bs}} \right) \qquad \text{Equation 5-47}$$

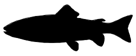
where

C_{sb} = COPC concentration sorbed to bed sediment (mg COPC/kg sediment)
f_{bs} = Fraction of total water body COPC concentration in benthic sediment (unitless)
C_{wtot} = Total water body COPC concentration, including water column and bed sediment (mg COPC/L water body)
Kd_{bs} = Bed sediment/sediment pore water partition coefficient (L COPC/kg water body)
θ_{bs} = Bed sediment porosity ($L_{\text{pore water}}/L_{\text{sediment}}$)
C_{BS} = Bed sediment concentration (g/cm^3)
d_{wc} = Depth of water column (m)
d_{bs} = Depth of upper benthic sediment layer (m)

We discussed f_{bs}, θ_{bs}, and C_{BS} in Section 5.7.4.1. We discussed C_{wtot}, d_{wc}, and d_{bs} in Section 5.7.4. We discuss Kd_{bs} in Appendix A-2.

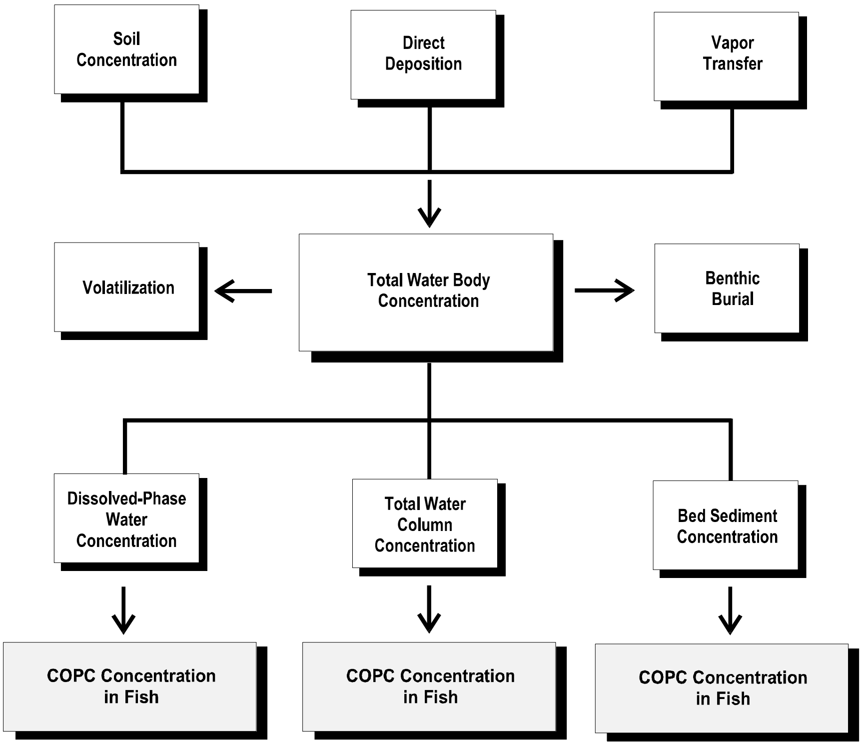
As in U.S. EPA (1994r) and NC DEHNR (1997), we continue to recommend using Equation 5-47 to calculate the COPC concentration sorbed to bed sediment.

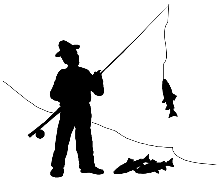
5.7.5 Concentration of COPC in Fish (C_{fish})



We generally recommend calculating the COPC concentration in fish using either a COPC-specific bioconcentration factor (*BCF*), a COPC-specific bioaccumulation factor (*BAF*), or a COPC-specific biota-sediment accumulation factor (*BSAF*). Under this approach you would use *BCFs* for COPCs with a $log\ K_{ow}$ less than 4.0. We assume that COPCs with a $log\ K_{ow}$ greater than 4.0 (except for extremely hydrophobic compounds such as dioxins, furans, and PCBs), have a high tendency to bioaccumulate. As a result, *BAF*s are used. While we assume that extremely hydrophobic COPCs like dioxins, furans, and PCBs also have a high tendency to bioaccumulate, they are expected to be sorbed to the bed sediments more than associated with the water phase. Therefore, we recommend using *BSAF*s to calculate concentrations of dioxins, furans, and PCBs in fish. Appendix A-2 provides a detailed discussion on the sources of the COPC-specific *BCF*, *BAF*, and *BSAF* values, and the method we used to derive them.

FIGURE 5-8
COPC CONCENTRATION IN FISH





BCF and *BAF* values are generally based on dissolved water concentrations. Therefore, when you use *BCF* or *BAF* values, it's appropriate to calculate the COPC concentration in fish using dissolved water concentrations. *BSAF* values are based on benthic sediment concentrations. Therefore, when using *BSAF* values, we recommend calculating COPC concentrations in fish using benthic sediment concentrations. We describe our recommended equations for calculating fish concentrations in the subsequent subsections.

5.7.5.1 Fish Concentration (C_{fish}) from Bioconcentration Factors Using Dissolved Phase Water Concentration

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-48 to calculate fish concentration from *BCF*s using dissolved phase water concentration. Using this equation is further described in Appendix B, Table B-4-26.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Bioconcentration Factors (BCF_{fish})
Using Dissolved Phase Water Concentration

$$C_{fish} = C_{dw} \cdot BCF_{fish}$$ Equation 5-48

where

C_{fish} = Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{dw} = Dissolved phase water concentration (mg COPC/L)
BCF_{fish} = Bioconcentration factor for COPC in fish (L/kg)

We discussed C_{dw} in Section 5.7.4.9. COPC-specific BCF_{fish} values are presented in the HHRAP companion database.

5.7.5.2 Fish Concentration (C_{fish}) from Bioaccumulation Factors Using Dissolved Phase Water Concentration

We recommend using Equation 5-49 to calculate fish concentration from *BAF*s using dissolved phase water concentration. The equation is also presented in Appendix B, Table B-4-27.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Bioaccumulation Factors (BAF_{fish})
Using Dissolved Phase Water Concentration

$$C_{fish} = C_{dw} \cdot BAF_{fish} \qquad \text{Equation 5-49}$$

where

C_{fish} = Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{dw} = Dissolved phase water concentration (mg COPC/L)
BAF_{fish} = Bioaccumulation factor for COPC in fish (L/kg FW tissue)

We discussed C_{dw} in Section 5.7.4.9. COPC-specific bioaccumulation factor (BAF_{fish}) values are presented in the HHRAP companion database.

5.7.5.3 Fish Concentration (C_{fish}) from Biota-To-Sediment Accumulation Factors Using COPC Sorbed to Bed Sediment

As in U.S. EPA (1994r) and NC DEHNR (1997), we recommend using Equation 5-50 to calculate fish concentration from *BSAF*s using COPC concentrations sorbed to bed sediment. We recommend using *BSAFs* for very hydrophobic compounds such as dioxins, furans, and PCBs. The equation is also presented in Appendix B, Table B-4-28.

Recommended Equation for Calculating:
Fish Concentration (C_{fish}) from Biota-To-Sediment Accumulation Factors *(BSAF)*
Using COPC Sorbed to Bed Sediment

$$C_{fish} = \frac{C_{sb} \cdot f_{lipid} \cdot BSAF}{OC_{sed}} \qquad \text{Equation 5-50}$$

where

C_{fish} = Concentration of COPC in fish (mg COPC/kg FW tissue)
C_{sb} = Concentration of COPC sorbed to bed sediment (mg COPC/kg bed sediment)
f_{lipid} = Fish lipid content (unitless)
$BSAF$ = Biota-to-sediment accumulation factor (unitless)
OC_{sed} = Fraction of organic carbon in bottom sediment (unitless)

We discussed C_{sb} in Section 5.7.4.10. We discuss f_{lipid} and OC_{sed} below. Our recommended default values for f_{lipid} and OC_{sed} are given in Appendix B, Table B-4-28. We offer biota-to-sediment accumulation factors (*BSAF*), which are applied only to dioxins, furans, and PCBs, in the HHRAP companion database.

Values recommended by U.S. EPA (1998c) range from 0.03 to 0.05 for $_{OCSED}$. These values are based on an assumption of a surface soil organic carbon (OC) content of 0.01. U.S. EPA (1998c) states that the organic carbon content in bottom sediments is higher than the organic carbon content in soils because (1) erosion favors lighter-textured soils with higher organic carbon contents, and (2) bottom sediments are partially comprised of detritus materials.

The fish lipid content (f_{lipid}) value is site-specific and dependent on the type of fish consumed. As stated in Appendix B, Table B-4-28, we recommend a default range of 0.03 to 0.07 specific to warm or cold water fish species. U.S. EPA (2000c) provides information supporting a value of 0.03 (3 percent lipid content of the edible portion). U.S. EPA (1993e) recommended a default value of 0.04 for $_{OCSED}$, which is the midpoint of the specified range. U.S. EPA (1993f; 1993e) recommended using 0.07, which was originally cited in Cook et al. (1991).

5.8 USING SITE-SPECIFIC vs. DEFAULT PARAMETER VALUES

As initially discussed in Chapter 1, many of the parameter values we recommend in the HHRAP are not site-specific. After completing a risk assessment using HHRAP default values, you might choose to investigate using site-specific parameter values. More site-specific values might provide a more representative estimate of site-specific risk. If you use parameter values other than those specified in the HHRAP, we recommend that you clearly described them in the risk assessment report. We also recommend that you discuss them with the permitting authority prior to using them. We recommend that requests to change default parameter values include the following information, as appropriate:

1. An explanation of why using a more site-specific parameter value is warranted (e.g., the default parameter is based on data or studies at sites in the northwestern U.S., but the facility is located in the southeast);
2. The technical basis of the site-specific parameter value, including readable copies of any relevant technical literature or studies;

3. A comparison of the weight-of-evidence between the competing studies (e.g., the site-specific parameter value is based on a study that is more representative of site conditions, a specific exposure setting being evaluated, or a more scientifically valid study than the default parameter, the site-specific parameter is based on the analysis of 15 samples as opposed to 5 for the default parameter, or the site-specific study used more stringent quality control/quality assurance procedures than the study upon which the default parameter is based);

4. A description of other risk assessments or projects that used the site-specific parameter value, and how such risk assessments or projects are similar to the current risk assessment.

RECOMMENDED INFORMATION FOR RISK ASSESSMENT REPORT

7 Identification of site-specific or alternate default media equations and/or inputs; including justification and full referencing

7 Media concentration calculations

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