Equations for Evaluating Exposure and Risk

1.0   ESTIMATION OF MEDIA CONCENTRATIONS

The purpose of this section is to present the media concentration estimation equations and associated parameters used in evaluation of the recommended exposure scenarios in Section 5.0 of this protocol, Exposure Assessment. Derivations of the equations are found in Appendix B of the HHRAP guidance (USEPA, 2005) and are not presented in this section. The equations are organized according to exposure pathway. References made throughout this section to particle phase are generic and made without distinction between particle phase and particle-bound phase.

Subsection 1.1 describes the equations used to estimate COPC air concentration. These air concentrations are the basis for acute and chronic COPC exposure via direct inhalation. Subsections 1.2 through 1.7 describe the equations used to estimate COPC concentrations in various media other than air. These media concentrations are the basis for chronic indirect COPC exposure via ingestion of potentially contaminated media.

Chapter 2.0 describes how the total potential exposure to COPCs is quantified based on estimated media concentrations.

1.1   Calculation of COPC Concentrations in Air for Direct Inhalation

COPC concentrations in air are calculated by summing the vapor phase and particle phase air concentrations of COPCs.

1.1.1   Calculation of COPC Concentrations in Air for Direct Inhalation via Long-term (Chronic) Exposure

$$C_a \quad = \quad Q \cdot \left[F_v \cdot Cyv + \left(1.0 - F_v \right) \cdot Cyp \right]$$

Where:

C_a	=	Air concentration ($\mu g/m^3$)
Q	=	COPC-specific emission rate (g/s)
Cyv	=	Unitized yearly air concentration from vapor phase (μg-s/g-m^3)
Cyp	=	Unitized yearly air concentration from particle phase (μg-s/g-m^3)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)

The fraction of COPC air concentration in the vapor phase (F_v) is COPC specific. Both the unitized yearly air concentration from vapor phase (Cyv) and the unitized yearly air concentration from particle phase (Cyp) are determined by the dispersion model.

1.1.2 Calculation of COPC Concentrations in Air for Direct Inhalation via Short-term (Acute) Exposure

$$C_{acute} \quad = \quad Q \cdot \left[F_v \cdot C_{hv} + \left(1.0 - F_v \right) \cdot C_{hp} \right]$$

Where:

C_{acute}	=	Acute air concentration ($\mu g/m^3$)
Q	=	COPC-specific emission rate (g/s)
C_{hv}	=	Unitized hourly air concentration from vapor phase ($\mu g\text{-}s/g\text{-}m^3$)
C_{hp}	=	Unitized hourly air concentration from particle phase ($\mu g\text{-}s/g\text{-}m^3$)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)

The fraction of COPC air concentration in the vapor phase (F_v) is COPC specific. Both the unitized hourly air concentration from vapor phase (Chv) and the unitized yearly air concentration from particle phase (Chp) will be determined by the dispersion model.

1.1.3 Calculation of Elemental and Divalent Mercury Concentration in Air for Direct Inhalation

The HHRAP provides mercury-specific equations that are functions of the total mercury emission rate. To account for mercury speciation and the global mercury cycle, the total mercury emission rate is multiplied by a factor of 0.002 for elemental mercury or by a factor of 0.48 for divalent mercury. Derivation of these factors is illustrated by Figure 2-4 of the HHRAP. Vapor phase oxidized mercury and particle-bound mercury are assumed to be in the form of divalent mercury (Hg2). To account for the global mercury cycle, total mercury emission rates are multiplied by the following factors: 1% for elemental mercury, 68% vapor phase divalent mercury, and 36% of particle-bound divalent mercury.

The modified mercury-specific equations for the calculation of elemental and divalent mercury air concentrations are presented below.

For elemental mercury:

$$C_{a\_Hg0} = 0.01 \cdot Q_{Hg0} \cdot Cyv$$

$$C_{acute\_Hg0} = 0.01 \cdot Q_{Hg0} \cdot C_{hv}$$

Elemental mercury is evaluated only for the inhalation exposure pathway. Acute air concentration for elemental mercury is the only species of mercury evaluated for the acute inhalation exposure pathway.

For divalent mercury:

$$C_{a\_Hg2} = f_{Hg2} \cdot Q_{Hg2} \cdot \left[F_{v\_Hg2} \cdot Cyv + \left(1.0 - F_{v\_Hg2} \right) \cdot Cyp \right]$$

$$C_{acute\_Hg2} = f_{Hg2} \cdot Q_{Hg2} \cdot \left[F_{v\_Hg2} \cdot Chv + \left(1.0 - F_{v\_Hg2} \right) \cdot Chp \right]$$

where,

$$Q_{Hg2} = Q_{Hg2\_v} + Q_{Hg2\_pb}$$

$$f_{Hg2} = \frac{0.68 \cdot Q_{Hg2\_v} + 0.36 \cdot Q_{Hg2\_pb}}{Q_{Hg2}}$$

$$F_{v\_Hg2} = \frac{0.68 \cdot Q_{Hg2\_v}}{0.68 \cdot Q_{Hg2\_v} + 0.36 \cdot Q_{Hg2\_pb}}$$

The subscripts Hg2_v, and Hg2_pb designate between vapor phase divalent mercury and particle bound phase divalent mercury, respectively.

1.2 Calculation of COPC Concentrations in Soil

COPC concentrations in soil are calculated by summing the vapor phase and particle phase deposition of COPCs to the soil. Wet and dry deposition of particles and vapors are considered, with dry deposition of vapors calculated from the vapor air concentration and the dry deposition velocity. The calculation of soil concentration incorporates a term that accounts for loss of COPCs by several mechanisms, including leaching, erosion, runoff, degradation (biotic and abiotic), and volatilization. These loss mechanisms all lower the soil concentration associated with the deposition rate. Equations for the calculation of soil concentration and soil losses of COPCs are presented in Appendix B of the HHRAP guidance document, Table B-1 for general soil , and Table B-4 for watershed soils.

Soil concentrations may require many years to reach steady state. As a result, the equations used to calculate the average soil concentration over the period of deposition only derived by integrating the instantaneous soil concentration over the period of deposition.

Soil conditions- such as pH, structure organic matter content, and moisture content- affect the distribution and mobility of COPCs. Loss of COPCs from the soil is modeled by using rates that depend on the physical and chemical characteristics of the soil. These variables and their use are described in the following subsections, along with the recommended equations.

1.2.1 Calculation of Cumulative Soil Concentration

Cumulative Soil Concentration (Cs) is calculated using one of the following three equations, depending upon the carcinogenicity of the COPC, and the time period of deposition:

Carcinogens:

For $T_2 \leq tD$

$$Cs = \frac{Ds}{ks \cdot (tD - T_1)} \cdot \left[\left(tD + \frac{\exp(-ks \cdot tD)}{ks} \right) - \left(T_1 + \frac{\exp(-ks \cdot T_1)}{ks} \right) \right]$$

For $T_1 < tD < T_2$

$$Cs = \frac{\left(\dfrac{Ds \cdot tD - Cs_{tD}}{ks} \right) + \left(\dfrac{Cs_{tD}}{ks} \right) \cdot \left(1 - \exp[-ks \cdot (T_2 - tD)] \right)}{(T_2 - T_1)}$$

Noncarcinogens:

$$Cs_{tD} = \frac{Ds[1 - \exp(-ks \cdot tD)]}{ks}$$

Where:

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Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Ds	=	Deposition term (mg COPC/kg soil/yr)
T_1	=	Time period at the beginning of combustion (yr)
ks	=	COPC soil loss constant due to all processes (yr^{-1})
tD	=	Time period over which deposition occurs (time period of combustion)
Cs_{tD}	=	Soil concentration at time tD (mg/kg)
T_2	=	Length of exposure duration (yr)

1.2.2   Calculation of the COPC Soil Loss Constant

Organic and inorganic COPCs may be lost from the soil by several processes that may or may not occur simultaneously. The rate at which a COPC is lost from the soil is known as the soil loss constant (*ks*). The constant ks is determined by using the soil's physical, chemical, and biological characteristics to consider the loss resulting from:

(1) leaching
(2) runoff
(3) erosion
(4) biotic and abiotic degradation
(5) volatilization

Because COPC loss from soil depends on many complex factors, it may be difficult to model the overall rate of loss. In addition, because the physical phenomena that cause COPC loss can occur simultaneously, the use of this equation may also overestimate loss rates for each process.

$$ks = ksg + kse + ksr + ksl + ksv$$

Where:

ks	=	COPC soil loss constant due to all processes (yr^{-1})
ksg	=	COPC loss constant due to biotic and abiotic degradation (yr^{-1})
kse	=	COPC loss constant due to soil erosion (yr^{-1})
ksr	=	COPC loss constant due to surface runoff (yr^{-1})
ksl	=	COPC loss constant due to leaching (yr^{-1})
ksv	=	COPC loss constant due to volatilization

COPC loss constant due to biotic and abiotic degradation (*ksg*) is COPC specific. A value of zero will be given to COPC loss constant due to soil erosion (*kse*) as recommended in section 5.2.2.2 of the HHRAP guidance. The following paragraphs discuss issues associated with the calculation of the *ksr*, *ksl*, and *ksv* variables.

1.2.3   Calculation of the COPC Loss Constant Due to Runoff, Leaching and Volatilization

The following equation will be used for calculating COPC loss due to runoff (k_{sr}):

$$ksr = \frac{RO}{\theta_{SW} \cdot Z_S} \cdot \left(\frac{1}{1 + \left(Kd_s \cdot BD / \theta_{SW} \right)} \right)$$

Where:

ksr	=	COPC loss constant due to runoff (yr^{-1})
RO	=	Average annual surface runoff from pervious areas (cm/yr)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (mL water/g soil)
BD	=	Soil bulk density (g soil/cm^3 soil)

The soil mixing zone depth (Z_s) is 2 cm for untilled soil and 20 cm for tilled soil as given in section 5.2.4.1 of the HHRAP. The recommended value for soil dry bulk density (*BD*) is 1.50 g/cm^3 as given in section 5.2.4.2 of the HHRAP. Soil volumetric water content (θ_{sw}) is 0.2 mL water/cm^3 as given in section 5.2.5.4 of the HHRAP. The average annual surface runoff from pervious areas (*RO*) will be determined for the assessment. The soil-water partition coefficient (Kd_s) for is COPC specific.

The following equation will be used to calculate COPC loss constant due to leaching (*ksl*):

$$ksl = \frac{P + I - RO - E_v}{\theta_{SW} \cdot Z_S \cdot \left[1.0 + \left(BD \cdot Kd_s / \theta_{SW} \right) \right]}$$

Where:

ksl	=	COPC loss constant due to leaching (yr^{-1})
P	=	Average annual precipitation (cm/yr)
I	=	Average annual irrigation (cm/yr)

RO	=	Average annual surface runoff from pervious areas (cm/yr)
E_v	=	Average annual evapotranspiration (cm/yr)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Z_s	=	Soil mixing zone depth (cm)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
BD	=	Soil bulk density (g soil/cm^3 soil)

The soil mixing zone depth (Z_s) is 2 cm for untilled soil and 20 cm for tilled soil as given in section 5.2.4.1 of the HHRAP. Soil volumetric water content (θ_{sw}) is 0.2 mL water/cm^3 as given in section 5.2.4.4 of the HHRAP. The recommended value for soil dry bulk density (BD) is 1.50 g/cm^3 as given in section 5.2.4.2 of the HHRAP. The soil-water partition coefficient (Kd_s) for is COPC specific. The average annual surface runoff from pervious areas (RO) will be determined for the assessment area. The average annual precipitation (P) is approximately 224 cm/yr (http://www.info.gov.hk/info/hkbrief/eng/fact.htm),

Semi-volatile and volatile COPCs emitted in high concentrations may become adsorbed to soil particles and exhibit volatilization losses from soil. The loss of a COPC from the soil by volatilization depends on the rate of movement of the COPC to the soil surface, the chemical vapor concentration at the soil surface, and the rate at which vapor is carried away by the atmosphere (Jury 1986).

U.S. EPA (1990e) recommended the use of Equation 5-6 of the HHRAP to calculate the constant for the loss of soil resulting from volatilization (ksv).

$$ksv = Ke \cdot Kt$$

Where:

ksv	=	COPC loss constant due to volatization (yr^{-1})
Ke	=	Equilibrium coefficient (s/cm-yr)
Kt	=	Gas phase mass transfer coefficient (cm/s)

The equilibrium coefficient (Ke) is calculated using the following equation:

$$Ke = \frac{3.1536E + 7 \cdot H}{Z_s \cdot K_{ds} \cdot R \cdot T \cdot BD}$$

Where:

| Ke | = | equilibrium coefficient (s/yr-cm) |

3.1536E+7=		unit conversion factor ([3.1536E+7 s/yr])
H	=	Henry's Law constant (atm-m^3/mol)
Z_s	=	soil mixing zone depth (cm)
K_{ds}	=	Soil-water partition coefficient (cm^3 water/g soil)
R	=	ideal gas constant (atm-m^3/mol-K)
T	=	temperature (K)
BD	=	bulk density of soil (g/cm^3)

Henry's Law constant (*H*) and the soil-water partition coefficient (K_{ds}) are COPC specific. The soil mixing zone depth (Z_s) is 2 cm for untilled soil and 20 cm for tilled soil as given in section 5.2.4.1 of the HHRAP. The ideal gas constant (*R*) is 8.205E-5 atm-m^3/mol-K and the temperature (T) is 298 K. The recommended value for soil dry bulk density (*BD*) is 1.50 g/cm^3 as given in section 5.2.4.2 of the HHRAP.

The gas-phase transfer coefficient (K_t) is based on the general soil properties (Hillel, 1980; Miller and Gardiner, 1998) which can be used to calculate the following equation:

$$K_t = \frac{D_a \cdot \theta_v}{Z_s}$$

where:

K_t	=	gas-phase mass transfer coefficient (cm/s)
Z_s	=	soil mixing depth (cm)
D_a	=	diffusion coefficient of contaminant in air (cm^3/s)
θ_v	=	soil void fraction (cm^3/cm^3)

The diffusion coefficient of contaminant in air (D_a) is COPC specific. The soil mixing zone depth (Z_s) is 2 cm for untilled soil and 20 cm for tilled soil as given in section 5.2.4.1 of the HHRAP.

The soil void fraction (θ_v) is the volumetric fraction of soil that does not contain solids or water and is calculated as follows:

$$\theta_v = 1 - (\frac{BD}{\rho_s}) - \theta_{sw}$$

where:

BD	=	soil bulk density (g/cm^3) – 1.5 g/cm^3
ρ_s	=	solids particle density (g/cm^3) – 2.7 g/cm^3

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The volumetric soil water content (θ_{sw}) is 0.2 mL/cm^3 as given. The recommended value for soil dry bulk density (BD) is 1.50 g/cm^3 as given in section 5.2.4.2 of the HHRAP. The solids particle density () is 2.7 g/cm^3.

1.2.4 Calculation of the Deposition Term

The following equation will be used to calculate the deposition term (Ds).

$$Ds = \left[\frac{100 \cdot Q}{Z_s \cdot BD}\right] \cdot \left[F_v \cdot (0.31536 \cdot Dydv + Dywv) + (Dydp + Dywp) \cdot (1 - F_v)\right]$$

Where:

Ds	=	Deposition term (mg COPC/kg soil/yr)
100	=	Units conversion factor (mg-m^2/kg-cm^2)
Q	=	COPC emission rate (g/s)
Z_s	=	Soil mixing zone depth (cm)
BD	=	Soil bulk density (g soil/cm^3 soil)
F_v	=	Fraction of COPC air concentration from vapor phase (m-g-s/g-m^3)
0.31536	=	Units conversion factor (m-g-s/cm-ug-yr)
$Dydv$	=	Dry deposition velocity (s/m2-yr)
$Dywv$	=	Unitized average yearly wet deposition from vapor phase (s/m^2-yr)
$Dydp$	=	Unitized average yearly dry deposition particle phase (s/m^2-yr)
$Dywp$	=	Unitized yearly wet deposition from particle phase (s/m^2-yr)

The fraction of COPC air concentration in the vapor phase (F_v) is COPC specific. The soil mixing zone depth (Z_s) is 2 cm for untilled soil and 20 cm for tilled soil as given in section 5.2.4.1 of the HHRAP. The recommended value for soil dry bulk density (BD) is 1.50 g/cm^3 as given in section 5.2.4.2 of the HHRAP.

1.3 Calculation of COPC Concentrations in Produce

Three possible mechanisms exist for contamination of aboveground exposed produce. They are described in the following equation.

Calculation of COPC Concentrations in Produce

$$C_{prod} = Pd + Pv + Pr$$

Where:

C_{prod}	=	Total COPC concentration in aboveground exposed produce (mg COPC/kg produce)
Pd	=	Concentration of COPC in the plant (aboveground produce) due to direct (wet and dry) deposition (mg COPC/kg DW)
Pv	=	Concentration of COPC in the plant resulting from air-to-plant transfer (ug COPC/g DW)
Pr	=	Total produce concentration due to root uptake (mg/kg)

1.3.1 Aboveground Produce Concentration Due to Direct Deposition

As recommended in the HHRAP, the following equation will be used to calculate the aboveground produce concentration due to direct deposition (Pd):

$$Pd = \frac{1000 \cdot Q \cdot (1 - F_V) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)]}{Yp \cdot kp}$$

Where:

Pd	=	Plant (aboveground produce) concentration due to direct (wet and dry) deposition (mg COPC/kg DW)
$1,000$	=	Units conversion factor (mg/kg)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
$Dydp$	=	Unitized yearly average dry deposition from particle-bound phase (s/m^2-yr)
Fw	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$Dywp$	=	Unitized yearly wet deposition from particle-bound phase
Rp	=	Interception fraction of the edible portion of plant (unitless)
kp	=	Plant surface loss coefficient (yr^{-1})
Tp	=	Length of plant exposure to deposition per harvest of the edible portion of the ith plant group (yr)
Yp	=	Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m^2)

The fraction of COPC air concentration in the vapor phase (F_v) is COPC specific. The fraction of COPC wet deposition that adheres to plant surfaces (Fw) is 0.2 for most anion COPCs and 0.6 for cations and most organic COPCs. The recommended value for the interception fraction of the edible portion of plant (Rp) is 0.39 given in section 5.3.1.1 of the

HHRAP. The plant surface loss coefficient (*Kp*) is 18, given by section 5.3.1.2 of the HHRAP. The length of plant exposure to deposition per harvest of edible portion of plant (*Tp*) is 0.164 given in section 5.3.1.3 of the HHRAP. The recommended value for standing crop biomass (*Yp*) is 2.24, given in section 5.3.1.4 of the guidance.

1.3.2 Aboveground Produce Concentration Due to Air-to-Plant Transfer

The following equation will be used to calculate the aboveground produce concentration due to air-to-plant transfer (*Pv*):

$$Pv \quad = \quad Q \cdot F_V \cdot \frac{Cyv \cdot Bv_{ag} \cdot VG_{ag}}{\rho_a}$$

Where:

Pv	=	Concentration of COPC in the plant resulting from air-to-plant transfer (µg COPC/g DW)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Cyv	=	Unitized yearly average air concentration from vapor phase (µg-s/g-m^3)
Bv_{ag}	=	COPC air-to-plant biotransfer factor ([mg COPC/g DW plant]/[mg COPC/g air]) (unitless)
VG_{ag}	=	Empirical correction factor for aboveground produce (unitless)
ρ_a	=	Density of air (g/m^3)

The fraction of COPC air concentration in the vapor phase (F_v), the COPC air-to-plant biotransfer factor (Bv_{ag}), and the empirical correction factor for aboveground produce (VG_{ag}) are COPC specific. VG_{ag} is 0.01 for COPC with log(K_{ow}) > 4 and 1.0 for COPC with log(K_{ow}) < 4. The density of air is 1200.00 as given in Table B-2-8 of the HHRAP.

1.3.3 Produce Concentration Due to Root Uptake

Following HHRAP recommendations, the produce concentration due to root uptake (*Pr*) will be calculated using the following equation:

$$Pr \quad = \quad Pr_a + Pr_b$$

Where:

Pr	=	Total produce concentration due to root uptake (mg/kg)
Pr_a	=	Produce concentration due to root uptake from exposed and protected produce (mg/kg).
Pr_b	=	Produce concentration due to root uptake from belowground produce (mg/kg)

To calculating the produce concentration due to root uptake from exposed and protected aboveground produce (Pr_{ag}), the following equation will be used:

$$Pr_{ag} = Cs \cdot Br_{ag}$$

Where:

Pr_{ag}	=	Produce concentration due to root uptake from exposed and protected produce (mg/kg).
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Br_{ag}	=	Plant-soil bioconcentration factor for produce (unitless)

The plant-soil bioconcentration factor for produce (Br_{ag}) is COPC specific.

The following equation will be used to calculate the produce concentration due to root uptake from belowground produce (Pr_{bg}):

$$Pr_{bg} = \frac{Cs \cdot VG_{rootveg} \cdot Br_{rootveg}}{1\ kg\ /\ L}$$

Where:

Pr_{bg}	=	Produce concentration due to root uptake from below ground produce (mg/kg).
$Br_{vootreg}$	=	Plant-soil bioconcentration factor for produce (unitless)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
$VG_{rootveg}$	=	Empirical correction factor for belowground produce (unitless)

The plant-soil bioconcentration factor for produce ($Br_{vootreg}$) is COPC specific. $VG_{rootveg}$ is 0.01 for COPC with log (K_{ow}) > 4 and 1.0 for COPC with log (K_{ow}) < 4.

1.4   Calculation of COPC Concentrations in Beef and Dairy Products

Concentrations of COPCs in beef and milk are estimated based on cattle diet, which consists of forage, silage, and grain. The routes of contamination to these feed streams are by direct deposition, vapor transfer and uptake through roots.

1.4.1 Forage and Silage Concentrations Due to Direct Deposition

The forage and silage concentrations due to direct deposition are calculated using the equation presented in Section 5.3.1 for calculating aboveground produce concentration due to direct deposition:

$$Pd = \frac{1000 \cdot Q \cdot (1 - F_v) \cdot [Dydp + (Fw \cdot Dywp)] \cdot Rp \cdot [1.0 - \exp(-kp \cdot Tp)]}{Yp \cdot kp}$$

Where:

Pd	=	Plant (aboveground produce) concentration due to direct (wet and dry) deposition (mg COPC/kg DW)
$1,000$	=	Units conversion factor (mg/kg)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
$Dydp$	=	Unitized yearly average dry deposition from particle-bound phase (s/m^2-yr)
Fw	=	Fraction of COPC wet deposition that adheres to plant surfaces (unitless)
$Dywp$	=	Unitized yearly wet deposition from particle-bound phase
Rp	=	Interception fraction of the edible portion of plant (unitless)
kp	=	Plant surface loss coefficient (yr^{-1})
Tp	=	Length of plant exposure to deposition per harvest of the edible portion of the ith plant group (yr)
Yp	=	Yield or standing crop biomass of the edible portion of the plant (productivity) (kg DW/m^2)

Application of this equation differs from that presented in Section 5.3.1 in that it must be evaluated separately for forage and silage. Therefore, values for some of the variables are different. The fraction of COPC air concentration in the vapor phase (F_v) is COPC specific. The fraction of COPC wet deposition that adheres to plant surfaces (Fw) is 0.2 for most anion COPCs and 0.6 for cations and most organic COPCs. The recommended value for the interception fraction of the edible portion of plant (Rp) is 0.5 for forage and 0.46 for silage as given in section 5.4.1.1 of the HHRAP. The plant surface loss coefficient (Kp) is 18 given by

section 5.3.1.2 of the HHRAP. The length of plant exposure to deposition per harvest of edible portion of plant (*Tp*) is 0.12 for forage and 0.16 for silage as given in section 5.4.1.3 of the HHRAP. The recommended value for standing crop biomass (*Yp*) is 0.24 for forage and 0.8 for silage as given in section 5.4.1.4 of the HHRAP.

1.4.2 Forage and Silage Concentrations Due to Air-to-Plant Transfer

The forage and silage concentrations due to air-to-plant transfer are calculated using the equation presented in Section 5.3.2 of the HHRAP for calculating aboveground produce concentration due to air-to-plant transfer:

$$Pv = Q \cdot F_V \cdot \frac{Cyv \cdot Bv_{forage} \cdot VG_{ag}}{\rho_a}$$

Where:

Pv	=	Concentration of COPC in the plant resulting from air-to-plant transfer (µg COPC/g DW)
Q	=	COPC emission rate (g/s)
F_v	=	Fraction of COPC air concentration in vapor phase (unitless)
Cyv	=	Unitized yearly average air concentration from vapor phase (µg-s/g-m^3)
BV_{forage}	=	COPC air-to-plant biotransfer factor for forage and silage ([mg COPC/g DW plant]/[mg COPC/g air]) (unitless)
VG_{ag}	=	Empirical correction factor for aboveground produce (unitless)
ρ_a	=	Density of air (g/m^3)

Application of this equation differs from that presented in Section 5.3.2 in that it must be evaluated separately for forage and silage. Therefore, values for some of the variables are different. The fraction of COPC air concentration in the vapor phase (F_v) and the COPC air-to-plant biotransfer factor for forage and silage (Bv_{forage}) are COPC specific. The empirical correction factor for aboveground produce (VG_{ag}) is 1.00 as recommended by HHRAP, section 5.4.2.1. VG_{ag} is 1.0 for forage and 0.5 for silage. The density of air (ρ_a) is 1200.00 as given in Table B-3-8, of the HHRAP.

1.4.3 Forage, Silage and Grain Concentrations Due to Root Uptake

The forage, silage, and grain concentrations due to root uptake are calculated using the equation presented in Section 5.3.3 for calculating COPC concentration in aboveground produce due to root uptake:

$$Pr \quad = \quad Cs \cdot Br_{forage}$$

Where:

Pr = Concentration of COPC in forage/silage/grain due to root uptake (mg/kg)

Cs = Average soil concentration over exposure duration (mg COPC/kg soil)

Br_{forage} = Plant-soil bioconcentration factor for aboveground produce (unitless)

The plant-soil bioconcentration factor for produce (Br_{forage}) is COPC specific.

1.4.4 Beef Concentrations Resulting from Plant and Soil Ingestion

COPC concentrations in beef are dependent on the COPC concentrations contained in the plants and soil ingested by the beef. The COPC concentration in beef is calculated as follows:

$$A_{beef} \quad = \quad \left(\sum (F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{beef} \cdot MF$$

Where:

A_{beef} = Concentration of COPC in beef (mg COPC/kg FW tissue)

F_i = Fraction of plant type i grown on contaminated soil and ingested by the animal (cattle) (unitless)

Qp_i = Quantity of plant type i eaten by the animal (cattle) per day (kg DW plant/day)

P_i = Concentration of COPC in each plant type i eaten by the animal (cattle) (mg/kg DW)

Qs = Quantity of soil eaten by the animal (cattle) each day (kg/day)

Cs = Average soil concentration over exposure duration (mg COPC/kg soil)

Bs = Soil bioavailability factor (unitless)

Ba_{beef} = COPC biotransfer factor for beef (day/kg FW tissue)

MF = Metabolism factor (unitless)

The COPC biotransfer factor for beef (Ba_{beef}) is COPC specific. The recommended value for F_i is 1.0 as given in section 5.4.4.1 HHRAP. The quantity of plant type i eaten by the animal (cattle) each day (Qp_i) will be set to 8.8 kg DW/day for forage, 2.5 kg DW/day for silage, and

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0.47 kg DW/day for grain as given in section 5.4.4.2 of the HHRAP. The quantity of soil ingested by the animal (cattle) per day (Qs) is 0.5 kg/day as given in section 5.4.4.4 of the HHRAP. The soil bioavailability factor (Bs) is 1.0 as given in section 5.4.4.6 of the guidance. The metabolism factor (MF), as given in section 5.4.4.7 of the HHRAP is 1.0 for the potential COPCs identifies in Section 3.0 of this protocol.

1.4.5   COPC Concentration in Milk Due to Plant and Soil Ingestion

COPC concentrations in milk are calculated using the following equation:

$$A_{milk} \quad = \quad \left(\sum(F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs\right) \cdot Ba_{milk} \cdot MF$$

Where:

A_{milk}	=	Concentration of COPC in milk (mg COPC/kg FW milk)
F_i	=	Fraction of plant type i grown on contaminated soil and ingested by the animal (dairy cattle) (unitless)
Qp_i	=	Quantity of plant type i eaten by the animal (dairy cattle) per day (kg DW plant/day)
P_i	=	Concentration of COPC in each plant type i eaten by the animal (dairy cattle) (mg/kg DW)
Qs	=	Quantity of soil eaten by the animal (dairy cattle) each day (kg/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor (unitless)
Ba_{milk}	=	COPC biotransfer factor for milk (day/kg WW tissue)
MF	=	Metabolism factor (unitless)

The COPC biotransfer factor for milk (Ba_{milk}) is COPC specific. The recommended value for F_i is 1.0 as given in section 5.4.4.1 of the HHRAP. The quantity of plant type i eaten by the animal (dairy cattle) each day (Qp_i) will be set to 13.2 kg DW/day for forage, 4.1 kg DW/day for silage, and 3.0 kg DW/day for grain as given in section 5.4.5.2 of the HHRAP. The quantity of soil ingested by the animal (dairy cattle) per day (Qs) is 0.4 kg/day as given in section 5.4.5 of the HHRAP. The soil bioavailability factor (Bs) as is 1.0 as given in section 5.4.4.6 of the HHRAP. The metabolism factor (MF), as given in section 5.4.4.7 of the HHRAP is 1.0 for the potential COPCs identifies in Section 3.0 of this protocol.

1.5   Calculation of COPC Concentrations in Pork

Concentrations of COPCs in pork result from COPCs consumed through the swine's diet (silage and grain) and from COPCs contained in ingested soil. Calculation of the concentrations proceeds in a similar fashion to COPC concentration calculation in beef:

$$A_{pork} = \left(\sum (F_i \cdot Qp_i \cdot P_i) + Q_s \cdot Cs \cdot Bs \right) \cdot Ba_{pork} \cdot MF$$

Where:

A_{pork}	=	Concentration of COPC in pork (mg COPC/kg FW tissue)
F_i	=	Fraction of plant type i grown on contaminated
Qp_i	=	Quantity of plant type i eaten by the animal (swine) each day (kg DW plant/day)
P_i	=	Concentration of COPC in plant type i eaten by the animal (swine) (mg/kg DW)
Q_s	=	Quality of soil eaten by the animal (swine) (kg/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor for pork (day/kg FW tissue)
MF	=	Metabolism factor (unitless)

The COPC biotransfer factor for pork (Ba_{pork}) is COPC specific. The recommended value for F_i is identical to that for beef cattle as specified in Section 5.4.4.1 of the HHRAP. The quantity of plan type i eaten by the animal (swine) each day (Qp_i) will be summed for only silage and grain since forage is not eaten by silage. Grain ingestion rate will be set to 3.3 kg DW/day. Silage ingestion rate will be set to 1.4 kg DW/day. The quantity of soil eaten by the animal (swine) each day (Q_s) will be set to the recommended 0.37 kg DW/day from Section 5.5.4 of the HHRAP. The soil bioavailability factor (Bs) is given in Section 5.4.4.6 of the HHRAP. The metabolism factor (MF), as given in section 5.4.4.7 of the HHRAP is 1.0 for the potential COPCs identifies in Section 3.0 of this protocol.

1.6   Calculation of COPC Concentrations in Chicken and Eggs

COPC concentrations in chicken and eggs result from COPCs consumed through the ingestion of grain and soil. Ten percent of the chickens' diet is assumed to be soil, and the other 90 percent is assumed to be grain.

The following equation is used in calculating the concentration of COPCs in chicken

$$A_{chicken} = \left(\sum (F_i \cdot Qp_i \cdot P_i) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{chicken}$$

Where:

$A_{chicken}$	=	Concentration of COPC in chicken (mg COPC/kg FW tissue)
F_i	=	Fraction of plant type i grown on contaminated soil and ingested by the animal (chicken) (unitless)
Qp_i	=	Quantity of plant type i eaten by the animal (chicken) per day (kg DW plant/day)
P_i	=	Concentration of COPC in each plant type i eaten by the animal (chicken) (mg/kg DW)
Qs	=	Quantity of soil eaten by the animal (chicken) each day (kg/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor (unitless)
$Ba_{chicken}$	=	COPC biotransfer factor for chicken (day/kg FW tissue)

The COPC biotransfer factor for chicken ($Ba_{chicken}$) is COPC specific. The recommended value for F_i is 1.0 as given in section 5.4.4.1 of the HHRAP. The quantity of grain eaten by the chicken each day (Qp_i) will be set to 0.2 kg DW/day as given in section 5.6.1.2 HHRAP. The quantity of soil ingested by the animal (chicken) per day (Qs) is 0.022 kg/day as given in section 5.6.4 of the HHRAP. The soil bioavailability factor (Bs) as is 1.0 as given in section 5.4.4.6 of the HHRAP.

Calculating Concentration of COPC in Eggs

$$A_{egg} = \left(\sum \left(F_i \cdot Qp_i \cdot P_i \right) + Qs \cdot Cs \cdot Bs \right) \cdot Ba_{egg}$$

Where:

A_{egg}	=	Concentration of COPC in eggs (mg COPC/kg FW tissue)
F_i	=	Fraction of plant type i (grain) grown on contaminated soil and ingested by the animal (chicken) (unitless)
Qp_i	=	Quantity of plant type i (grain) eaten by the animal (chicken) per day (kg DW plant/day)
P_i	=	Concentration of COPC in each plant type i (grain) eaten by the animal (chicken) (mg/kg DW)
Qs	=	Quantity of soil eaten by the animal (chicken) each day (kg/day)
Cs	=	Average soil concentration over exposure duration (mg COPC/kg soil)
Bs	=	Soil bioavailability factor (unitless)
Ba_{egg}	=	COPC biotransfer factor for eggs (day/kg FW tissue)

The COPC biotransfer factor for eggs (Ba_{egg}) is COPC specific. The recommended value for F_i is 1.0 as given in section 5.4.4.1 of the HHRAP. The quantity of plant type i eaten by the animal (chicken) each day (Qp_i) will be set to 0.2 as given in section 5.6.2 of the HHRAP. The quantity of soil ingested by the animal (chicken) per day (Qs) is 0.022 kg/day as given in section 5.6.4 of the HHRAP. The soil bioavailability factor (Bs) as is 1.0 as given in section 5.4.4.6 of the HHRAP.

1.7   Calculation of COPC Concentrations in Drinking Water and Fish

Determination of COPC concentrations in drinking water and fish are based on the COPC concentrations in the water body.

1.7.1   Calculation of COPC Load to the Water Body

Calculating Total COPC Load to the Water Body:

$$L_T \quad = \quad L_{DEP} + L_{DIF} + L_{RI} + L_R + L_E + L_I$$

Where:

L_T	=	Total COPC load to the water body (including deposition, runoff, and erosion) (g/yr)
L_{DEP}	=	Total (wet and dry) particle phase and wet vapor phase COPC direct deposition load to water body (g/yr)
L_{DIF}	=	Vapor phase COPC diffusion (dry deposition) load to water body (g/yr)
L_{RI}	=	Runoff load from impervious surfaces (g/yr)
L_R	=	Runoff load from pervious surfaces (g/yr)
L_E	=	Soil erosion load (g/yr)
L_I	=	Internal transfer (g/yr)

Internal transfer (L_I) will be set to zero as recommended in section 5.7.1 of the HHRAP. The equations for the variables L_{DEP}, L_{DIF}, L_{RI}, L_R, and L_E will be discussed below.

Calculating Total Particle Phase and Wet Vapor Phase Direct Deposition Load to Water Body:

$$L_{DEP} \quad = \quad Q \cdot [F_v \cdot Dywwv + (1 - F_v) \cdot Dytwp] \cdot A_w$$

Where:

L_{DEP} = Total (wet and dry) particle phase and wet 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)

$Dywwv$ = Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m²-yr)

$Dytwp$ = Unitized yearly (water body and watershed) average total (wet and dry) deposition from particle-bound phase (s/m²-yr)

A_w = Water body surface area (m²)

The fraction of COPC air concentration in the vapor phase (F_v) is COPC specific. The water body surface area (A_w) for the water bodies of interest will be determined.

Calculating Vapor Phase COPC Diffusion (Dry Deposition) Load to Water Body:

$$L_{dif} = \frac{K_V \cdot Q \cdot F_V \cdot Cywv \cdot A_W \cdot 1\times10^{-6}}{\dfrac{H}{R \cdot T_{WK}}}$$

Where:

L_{dif} = Vapor phase COPC diffusion (dry deposition) 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 and watershed) average air concentration from vapor phase (μg-s/g-m³)

A_W = Water body surface area (m²)

10^{-6} = Units conversion factor (g/μg)

H = Henry's Law constant (atm-m³/mol)

R = Universal gas constant (atm-m³/mol-K)

T_{WK} = Water body temperature (K)

Water body temperature (T_{WK}) is set to 298K as given in section 5.7.1.2 of the HHRAP. The fraction of COPC air concentration in the vapor phase (F_v) and Henry's Law constant (H) are COPC specific. The universal gas constant (R) is 8.205E-05. The water body surface area (A_w) for the water bodies of interest will be determined.

Calculating Runoff Load from Impervious Surfaces:

$$L_{RI} = Q \cdot [F_v \cdot Dywwv + (1.0 - F_v) \cdot Dytwp] \cdot A_I$$

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)

$Dywwv$ = Unitized yearly (water body and watershed) average wet deposition from vapor phase (s/m^2-yr)

$Dytwp$ = Unitized yearly (water body and watershed) average total (wet and dry) deposition from particle-bound phase (s/m^2-yr)

A_I = Impervious watershed area receiving COPC deposition (m^2)

The fraction of COPC air concentration in the vapor phase (F_v) is COPC specific. The impervious watershed area receiving COPC deposition (A_I) will be determined.

Calculating Runoff Load from Pervious Surfaces:

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

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)

θ_{sw} = Soil volumetric water content (mL water/cm^3 soil)

Kd_s = Soil-water partition coefficient (cm^3 water/g soil)

0.01 = Units conversion factor (kg-cm^2/mg-m^2)

The recommended value for soil dry bulk density (BD) is 1.50 g/cm^3 as given in section 5.2.4.2 of the HHRAP. Soil volumetric water content (θ_{sw}) is 0.2 ml/cm^3 as given in section 5.2.4.4 of the guidance. The soil-water partition coefficient (Kd_s) is COPC specific. Average annual surface runoff from pervious areas (RO) will be determined. The impervious

watershed area receiving COPC deposition (A_I) and the total watershed area (A_L) will be determined.

Calculating Soil Erosion Load:

$$L_E \quad = \quad X_e \cdot (A_L - A_I) \cdot SD \cdot ER \cdot \frac{Cs \cdot Kd_s \cdot BD}{\theta_{sw} + Kd_s \cdot BD} \cdot 0.001$$

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)
θ_{sw}	=	Soil volumetric water content (mL water/cm^3 soil)
Kd_s	=	Soil-water partition coefficient (cm^3 water/g soil)
0.001	=	Units conversion factor (kg-cm^2/mg-m^2)

The recommended value for soil dry bulk density (BD) is 1.50 g/cm^3 as given in section 5.2.4.2 of the HHRAP. Soil volumetric water content (θ_{sw}) is 0.2 ml/cm^3 as given in section 5.2.4.4 of the HHRAP. The soil-water partition coefficient (Kd_s) is COPC specific. The soil enrichment ratio (ER) is 1 for inorganics and 3 for organics as given in Table B-4-3, of the HHRAP). Average annual surface runoff from pervious areas (RO) will be determined. The impervious watershed area receiving COPC deposition (A_I) and the total watershed area (A_L) will be determined.

1.7.2   Universal Soil Loss Equation

The universal soil loss equation, shown below, is used to calculate the unit soil loss specific to each watershed:

$$X_e \quad = \quad RF \cdot K \cdot LS \cdot C \cdot PF \cdot (907.18 / 4047)$$

Where:

X_e	=	Unit soil loss (kg/m^2-yr)
RF	=	USLE rainfall (or erosivity) factor (yr^{-1})
K	=	USLE erodibility factor (ton/acre)

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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 inputs are generally site-specific and are described in greater detail in Table B-4-13 of the HHRAP guidance.

1.7.3 Sediment Delivery Ratio

The sediment delivery ratio for a watershed or part of a watershed is calculated based on the area of the watershed by using the following equation:

$$SD \quad = \quad a \cdot (A_L)^{-b}$$

Where:

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

The empirical slope coefficient (*b*) is 0.125 as given in section 5.7.3. of the HHRAP. The empirical intercept coefficient (*a*) is between 0.6 and 2.1, depending on watershed area.

1.7.4 Total Water Body COPC Concentration

The total water body concentration includes the COPC contributions from the water column and the sediment bed, as shown in the following equation:

$$C_{wtot} \quad = \quad \frac{L_T}{Vf_x \cdot f_{WC} + k_{wt} \cdot A_W \cdot \left(d_{WC} + d_{bs}\right)}$$

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)

Depth of upper benthic sediment layer (d_{bs}) is 0.03 as given in section 5.7.4 as given in the HHRAP. The average volumetric flow rate through water body (Vf_x) and the water body surface area (A_W) will be determined.

Calculating Fraction of Total Water Body COPC Concentration in the Water Column and Benthic Sediment.

$$f_{WC} = \frac{\left(1 + Kd_{sw} \cdot TSS \cdot 1x10^{-6}\right) \cdot d_{wc} / d_z}{\left[\left(1 + Kd_{sw} \cdot TSS \cdot 1x10^{-6}\right) \cdot d_{wc} / d_z + \left(\theta_{bs} + Kd_{bs} \cdot C_{BS}\right) \cdot d_{bs} / d_z\right]}$$

$$f_{bs} = 1 - f_{wc}$$

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)
$1 x 10^{-6}$	=	Units conversion factor (kg/mg)
d_z	=	Total water body depth (m)
θ_{bs}	=	Bed sediment porosity (Lwater / Lsediment)
Kd_{bs}	=	Bed sediment / sediment pore water partition coefficient (L water/kg bottom sediment)
C_{as}	=	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 suspended sediments/surface water partition coefficient (Kd_{sw}) and the bed sediment / sediment pore water partition coefficient (Kd_{bs}) are COPC specific. For total suspended solids concentration (TSS) will be determined on a site-specific basis. The bed sediment

porosity (θ_{bs}) is 0.6 as given in section 5.7.4.1 of the HHRAP. The depth of upper benthic sediment layer (d_{bs}) is 0.03 as given in Table B-4-16 of the HHRAP.

Calculating Overall Total Water Body COPC Dissipation Rate Constant:

$$k_{wt} \quad = \quad f_{WC} \cdot k_V + f_{bs} \cdot k_b$$

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})

Calculating Water Column Volatilization Rate Constant:

$$k_v \quad = \quad \frac{K_V}{d_Z \cdot \left(1 + Kd_{SW} \cdot TSS \cdot 1 \times 10^{-6}\right)}$$

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 suspended sediments/surface water partition coefficient (Kd_{sw}) is COPC specific. Total suspended solids concentration (TSS) will be determined on a site-specific basis.

Calculating Overall COPC Transfer Rate Coefficient:

$$Kv \quad = \quad \left(K_L^{-1} + \left(K_G \cdot \frac{H}{R \cdot T_{WK}}\right)^{-1}\right)^{-1} \cdot \theta^{T_{WK}-293}$$

Where:

Kv	=	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-m3/mol)
R	=	Universal gas constant (atm-m3/mol-K)
T_{wk}	=	Water body temperature (K)
θ	=	Temperature correction factor (unitless)

Water body temperature (T_{wk}) is set to 298K as given in section 5.7.1.2 of the HHRAP. Henry's Law constant (H) is COPC specific. The universal gas constant (R) is 8.205E-05. The temperature correction factor (θ) is 1.026 as given in section 5.7.4.4 of the HHRAP. The gas phase transfer coefficient (K_G) is 36,500 as given in section 5.7.4.6 of the HHRAP.

Calculating Liquid Phase Transfer Coefficient:

For streams and rivers -

$$K_L \quad = \quad \sqrt{\frac{\left(1\times10^{-4}\right)\cdot D_W \cdot u}{d_z}}\cdot 3.1536\times10^{-7}$$

For quiescent lakes and ponds –

$$K_L \quad = \quad \left(C_d{}^{0.5}\cdot W\right)\cdot\left(\frac{\rho_a}{\rho_w}\right)^{0.5}\cdot\frac{k^{0.33}}{\lambda_z}\cdot\left(\frac{\mu_W}{\rho_W \cdot D_W}\right)^{-0.67}\cdot 3.1536\times10^{7}$$

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)

The diffusivity of COPC in water (D_w) is COPC specific. The drag coefficient (C_d) is 0.0011 as specified in section 5.7.4.5 of the HHRAP. The average annual wind speed (W) is 3.9 m/s per Table B-4-20 of Appendix B of the HHRAP. The density of air (ρ_a) is 0.0012 g/cm^3, and the density of water (ρ_W) is 1 g/cm^3) as given in section 5.7.4.5 of the HHRAP. Von Karman's constant (k) is 0.4 (unitless), the dimensionless viscous sublayer thickness (λ_Z) is 4 (unitless), and the viscosity of water corresponding to water temperature (μ_W) is 0.0169 g/cm-s as given in section 5.7.4.5 of the HHRAP.

Calculating Benthic Burial Rate Constant:

$$k_b \quad = \quad \left(\frac{X_e \cdot A_L \cdot SD \cdot 1 \times 10^{-3} - Vf_X \cdot TSS}{A_W \cdot TSS} \right) \cdot \left(\frac{TSS \cdot 1 \times 10^{-6}}{C_{BS} \cdot d_{bs}} \right)$$

Where:

k_b	=	Benthic burial rate constant (yr-1)
X_e	=	Unit Soil loss (kg/m^2-yr)
A_L	=	Total watershed area 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)
1×10^{-6}	=	Units conversion factor (kg/mg)
1×10^3	=	Units conversion factor (g/kg)

Total suspended solids concentration (*TSS*), will be determined on a site-specific basis. The depth of upper benthic sediment layer (d_{bs}) is 0.03 as given in the HHRAP, Table B-4-16. The bed sediment concentration (C_{BS}) is 1.0 as given in section 5.7.4.8 of the HHRAP. The

total watershed area receiving deposition (A_L), average volumetric flow rate through water body (V_{fx}) and water body surface area (A_W) will be determined.

Calculating Total COPC Concentration in Water Column:

$$C_{wctot} = f_{WC} \cdot C_{wtot} \cdot \frac{d_{WC} + d_{bs}}{d_{WC}}$$

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)

The depth of upper benthic sediment layer (d_{bs}) is 0.03 as given in Table B-4-16 of the HHRAP.

Calculating Dissolved Phase Water Concentration:

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{SW} \cdot TSS \cdot 1 \times 10^{-6}}$$

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)

The suspended sediments/surface water partition coefficient (Kd_{sw}) is COPC specific. Total suspended solids concentration (TSS) will be determined on a site-specific basis.

Calculating COPC Concentrations Sorbed to Bed Sediment:

$$C_{sb} \quad = \quad f_{bs} \cdot C_{wtot} \cdot \left(\frac{Kd_{bs}}{\theta_{bs} + Kd_{bs} \cdot C_{BS}} \right) \cdot \left(\frac{d_{WC} + d_{bs}}{d_{bs}} \right)$$

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 concentration ($L_{\text{pore water}}$/ L_{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)

The bed sediment/surface pore water partition coefficient (Kd_{bs}) is COPC specific. The depth of upper benthic sediment layer (d_{bs}) is 0.03 as given in Table B-4-16 of the HHRAP. The bed sediment concentration (C_{BS}) is 1.0 as given in section 5.7.4.8 of the HHRAP. The bed sediment / sediment pore water partition coefficient (θ_{bs}) is 0.6 as given in section 5.7.4.1 of the HHRAP.

1.7.5 Concentration of COPCs in Fish

The COPC concentrations in fish are calculated using either a COPC-specific bioconcentration factor (*BCF*), a COPC-specific biota-sediment accumulation factor (*BSAF*). In COPCs with a log k_{ow} less than 4.0, BCFs will be used. Compounds with a log k_{ow} greater than 4.0 (excluding extremely hydrophobic compounds) will tend to bioaccumulate, therefore, BAFs will be used. BSAF values will be used for extremely hydrophobic COPCs.

Calculating Fish Concentration from Bioconcentration Factors (BCF) Using Dissolved Phase Water Concentrations:

$$C_{fish} \quad = \quad C_{dw} \cdot BCF_{fish}$$

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 (kg) |

The dissolved phase water concentration (C_{dw}) calculation has been shown previously in this discussion. The BCF_{fish} values are COPC-specific.

Calculating Fish Concentration from Bioaccumulative Factors Using Dissolved Phase Water Concentration:

$$C_{fish} = C_{dw} \cdot BAF_{fish}$$

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)

The dissolved phase water concentration (Cdw) calculation has been shown previously in this discussion. The bioaccumulation factors (BAF_{fish}) are COPC-specific.

Calculating Fish Concentration from Biota-To-Sediment Accumulation Factors (BSAF) Using COPC Sorbed to Bed Sediment:

$$C_{fish} = \frac{C_{sb} \cdot f_{lipid} \cdot BSAF}{OC_{sed}}$$

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)

The biota-to-sediment accumulation factor ($BSAF$) is COPC specific. The fish lipid (f_{lipid}) content is 0.07, and the fraction of organic carbon in bottom sediment (OC_{sed}) is 0.04 as specified in Table B-4-28 of the HHRAP.

2.0 QUANTIFICATION OF EXPOSURE PROTOCOL

The calculation of Compound of Potential Concern (COPC) specific exposure rates for each exposure pathway involves (1) estimated COPC media concentrations calculated using the equations and methodologies previously presented in Section 5 of the protocol, Estimation of Media Concentrations, (2) consumption rate, (3) receptor body weight, and (4) the frequency and duration of exposure. This calculation will be repeated for each of the and for each exposure pathway included in an exposure scenario. Exposure pathway-specific equations are presented in Appendix C of the HHRAP. The following sections describe exposure rate calculations and the exposure pathway-specific variables, which may affect this calculation.

2.1 Generic Exposure Rate Equation

To calculate an average exposure per unit of time, the total exposure is divided by the time period. Average exposure can also be expressed in terms of body weight. All exposures quantified in the risk assessment (1) will be unitized for time and body weight, (2) will be presented in units of milligrams per kilogram of body weight per day, and (3) will be termed "intakes." The following equation is a generic equation used to calculate chemical intake.

$$I = \frac{C_{gen} \cdot CR \cdot EF \cdot ED}{BW \cdot AT}$$

Where:

I   =   Intake is the amount of COPC at the exchange boundary (mg/kg/day); for evaluating exposure to noncarcinogenic COPCs, the intake is referred to as average daily dose (ADD); for evaluating exposure to carcinogenic compounds, the intake is referred to as lifetime average daily dose (LADD)

C_{gen} =   Generic COPC concentration in media of concern (e.g., mg/kg for soil or mg/L for surface water);

CR   =   Consumption rate is the amount of contaminated medium consumed per unit of time or event (e.g., kg/day for soil and L/day for water)

EF   =   Exposure frequency (days/year)

ED   =   Exposure duration (years)

BW   =   Average body weight of the receptor over the exposure period (kg)

AT   =   Averaging time- the period over which exposure is averaged (days); for carcinogens, the averaging time is 25,550 days, based on a lifetime exposure of 70 years, for noncarcinogens, averaging time equals ED (years) multiplied by 365 days per year.

Variations of the generic equation will be used to calculate receptor-specific exposures to COPCs. The equations used for each exposure pathway are presented in Appendix C of the HHRAP. The variation of input variables when exposure is quantified is also described in Appendix C of the HHRAP.