APPENDIX C

Predictive Assessment Methods

1.0   PREDICTIVE ASSESSMENT METHODS

1.1   Calculating Exposure Point Concentrations

The following sections present the equations used to calculate the exposure point concentrations used in the Site Specific Human Health Risk Assessment (HHRA). Generally, the equations are given and the terms explained. Where site-specific values were used, rationale for these values is provided below. Where known standards or default values (as presented in US EPA, 2005) were adopted, these values are given in brackets. Unless otherwise stated, the equations presented are found in US EPA (2005).

1.1.1   Air

The following equation (US EPA, 2005) calculates the air concentration of a COPC based on the fraction in vapour phase and the fraction in particle phase.

$$C_a = \ Hg_{factorAl} \ x \ Q \ x \ [F_v \ x \ Cyv + (1.0 - F_v) \ x \ Cyp] \tag{1}$$

Where		Units
C_a=	Air Concentration	$\mu g/m^3$
Q=	COPC emission rate; discussed below	g/s
$Hg_{factorAl}$=	Mercury factor for air inhalation; discussed below	Unitless
F_v=	Fraction of COPC air concentration in vapor phase; COPC –specific	Unitless
Cyv=	Yearly air concentration from vapor phase	$\mu g/m^3$
Cyp=	Yearly air concentration from particle phase	$\mu g/m^3$

The $Hg_{factorAl}$ is 1.0 for all COPC, with the following exceptions:
- 0.002 for elemental mercury (Hg^0)
- 0.482 for divalent mercury (Hg^{2+})
- 0.0 for MHg

The yearly air concentration terms (Cyv and Cyp) and a COPC-specific emission rate (Q in g/s) are determined by air modelling, and are site- and COPC-specific. Note, for the purposes of this assessment, Q has been incorporated into the yearly concentration and deposition rates used in the model; therefore, Q, although presented in this equation and several that follow, was not actually used in the calculation (i.e., it was artificially set to 1.0). In addition, the data provided by the air modelers had also incorporated the Fv term. The equations are presented here to illustrate the general process; however, the actual methodology varies slightly depending on how the air data are provided.

1.2   Soil Concentration

Chemical concentrations in soil are calculated by summing the vapour and particle phase deposition of chemicals to the soil. The US EPA (2005) has recommended three different deposition equations depending on the duration of exposure and toxic mode of action. Two of the equations deal with carcinogenic chemicals and the third deals with all non-carcinogenic chemicals. The first equation is to be used if the exposure duration is less than the operating lifetime of the emission source or time period of combustion. The second equation should be

used when the exposure duration is greater than or equal to the operating lifetime of the emission source or period of combustion. The third equation is a variation of the first carcinogenic equation, which calculates the highest 1-year annual average soil concentration; typically occurring at the end of the operating life of the emission source (US EPA, 2005).

1.2.1 Carcinogen – soil concentration averaged over exposure duration

For $T_2 \leq tD$ – (exposure duration than or equal to the operating lifetime of the emission source):

$$C_S = \frac{D_S}{ks \times \left(tD - T_1\right)} \times \left[\left(tD + \frac{\exp\left(-ks \times tD\right)}{ks}\right) - \left(T_1 + \frac{\exp\left(-ks \times T_1\right)}{ks}\right)\right] + C_{s\,Background} \qquad (2)$$

For $T_1 < tD < T_2$ – (exposure duration less than or equal to the operating lifetime of the emission source):

$$C_S = \frac{\left(\dfrac{D_S \times tD - C_{StD}}{ks}\right) + \left(\dfrac{C_{StD}}{ks}\right) \times \left[1 - \exp\left[-ks \times \left(T_2 - tD\right)\right]\right]}{\left(T_2 - T_1\right)} + C_{s\,Background} \qquad (3)$$

1.2.2 Non-carcinogens maximum annual average soil concentrations

$$C_S = \frac{D_S \times \left[1 - \exp\left(-ks \times tD\right)\right]}{ks} \qquad (4)$$

Where		Units
$C_s =$	Average chemical soil concentration over exposure duration	mg/kg soil
$D_s =$	Deposition term; discussed below	mg chemical/kg soil/yr
$T_1 =$	Time period at the beginning of combustion	0 years
$Ks =$	Chemical soil less constant due to all processes; discussed below	yr^{-1}
$tD =$	Time period over which deposition occurs	30 year
$C_{stD} =$	Soil concentration at time tD (equivalent to C_s for non-carcinogens)	mg/kg
$T_2 =$	Length of exposure duration (applicable for carcinogens only)	75 year

The deposition term (D_s) is calculated as follows:

$$D_S = \left[\frac{100 \times Hg_{factor} \times Q}{Z_S \times BD}\right] \times \left[F_V \times \left(Dydv + Dywv\right) + \left(Dydp + Dywp\right) \times \left(1 - F_V\right)\right] \qquad (5)$$

Where		Units
D_s =	Deposition term	mg COPC/kg soil/yr
100 =	Units conversion factor	$mg\text{-}m^2/kg\text{-}cm^2$
$Hg_{factorDS}$ =	Mercury factor for deposition; discussed below	Unitless
Q=	COPC emission rate; discussed previously	g/s
Z_s =	Soil mixing zone depth	cm
BD =	Soil bulk density (15 g/cm^3)	g soil/cm^3 soil
F_v =	Fraction of COPC air concentration in vapour phase; COPC specific	unitless
Dydv =	Unitized yearly dry deposition from vapour phase; discussed below	s/m^2-yr
Dywv =	Unitized yearly wet deposition from vapour phase; discussed below	s/m^2-yr
Dydp =	Unitized yearly dry deposition from particle phase; discussed below	s/m^2-yr
Dywp =	Unitized yearly wet deposition from particle phase; discussed below	s/m^2-yr

The $Hg_{factorDS}$ for deposition is 1.0 for all COPCs, with the following exceptions:

- for Hg^0 (i.e., 0.482 * 0.0)
- 0.47236 for Hg^{2+} (i.e., 0.482 * 0.98)
- 0.00964 for MHg (i.e., 0.482 * 0.02)

In this risk assessment a 2cm mixing zone was employed to estimate soil concentrations and subsequent fate and transport of chemicals in the environment for all land uses.

The deposition terms (Dydv, Dywv, Dydp, and Dywp) are determined by air modelling and are site- and COPC-specific.

US EPA (2005) has outlined several processes through which chemicals may be lost from soil. These methods may or may not occur simultaneously. The total rate at which a chemical is lost from the soil is referred to as the soil loss constant (ks).

$$ks = ksg + kse + ksr + ksl + ksv \qquad (6)$$

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

The COPC loss constant due to biotic and abiotic degradation reflects the loss of a COPC from the soil by mechanisms other than leaching. Abiotic degradation includes photolysis, hydrolysis, and redox

reactions. Lyman et al. (1982) states that degradation rates can be assumed to follow first order kinetics in a homogeneous media.

(7)

$$kse = \frac{0.1 \times X_e \times SD \times ER}{BD \times Z_S} \times \frac{Kd_S \times BD}{\theta_{SW} + Kd_S \times BD}$$

Where:		Units
kse	COPC soil loss constant due to soil erosion	unitless
0.1	units conversion factor	$(1,000 \text{ g-kg}/10,000 \text{ cm}^2\text{-m}^2)$
X_e	unit soil loss; discussed below	$kg/m^2\text{-yr}$
SD	sediment delivery ratio; discussed below	unitless
ER	soil enrichment ratio; discussed below	unitless
BD	soil bulk density (1.5 g/cm^3)	$g \text{ soil}/cm^3 \text{ soil}$
Z_s	soil mixing zone depth; discussed previously	cm
Kd_s	soil/water partition coefficient; COPC- specific	mL water/g soil
θ_{sw}	soil volumetric water content (0.2 mL/cm^3)	$mL \text{ water}/cm^3 \text{ soil}$

The Unit Soil Loss Equation (USLE) is as follows:

(8)

$$X_e = RF \times K \times LS \times C \times PF \times \frac{907.18}{4047}$$

Where:		Units
RF	USLE rainfall (or erosivity) factor, site-specific	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 (1)	unitless
907.18	units conversion factor	kg/ton
4047	units conversion factor	$m^2/acre$

The sediment ratio is calculated as follows:

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

(9)

Where: Units

Appendix C – Predictive Assessment Methods

a	empirical intercept coefficient	unitless
A_L	total watershed area receiving deposition	m^2
b	empirical slope coefficient (0.125)	unitless

The empirical intercept coefficient (a), which varies by watershed area, and the total watershed area receiving deposition (A_L) are watershed-specific.

Recommended values for the soil enrichment ratio (ER) were adopted from US EPA (2005); 3 for organics, 1 for inorganics.

The loss constant due to surface runoff can be estimated using the following equation, as recommended by US EPA (2005):

$$ksr = \frac{RO}{\theta_{sw} \times Z_s} \times \left(\frac{1}{1 + Kd_s \times BD/\theta_{sw}} \right) \qquad (10)$$

Where: Units

ksr	COPC loss constant due to runoff	yr^{-1}
RO	average annual surface runoff from pervious areas; discussed below	cm/yr
θ_{sw}	soil volumetric water content (0.2 mL/cm^3)	mL water/cm^3 soil
Z_s	soil mixing zone depth; discussed previously	cm
Kd_s	soil/water partition coefficient; COPC-specific	mL water/g soil
BD	soil bulk density (1.5 g/cm^3)	g soil/cm^3 soil

The average annual surface runoff from pervious areas (RO) was 14.47 cm/yr, based on precipitation and evapotranspiration rates.

Losses of soil COPCs due to leaching (ksl) depend on the amount of water available to generate leachate and soil properties. The recommended equation for calculating ksl (US EPA, 2005) is as follows:

$$(11)$$

$$ksl = \frac{P + I - RO - E_v}{\theta_{sw} \times Z_s \times \left[1.0 + BD \times Kd_s/\theta_W \right]}$$

Where: Units

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 (0.2 mL/cm^3)	mL/cm^3

Z_s	soil mixing zone depth; discussed previously	cm
BD	soil bulk density (1.5 g/cm^3)	g soil/cm^3 soil
Kd_s	soil/water partition; COPC-specific	cm^3 water/g soil

The following climatological data was used in the assessment temperature, precipitation, humidity and wind direction.

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 vapour concentration at the soil surface, and the rate at which vapour is carried away by the atmosphere (Jury, 1986). The following equation is recommended by US EPA (2005) for calculating COPC loss constant due to volatilization:

(12)

$$ksv = \left(\frac{3.1536 \times 10^7 \times H}{Zs \times Kd_S \times R \times T_a \times BD} \right) \bullet \left(\frac{D_a}{Z_s} \right) \bullet \left[1 - \frac{BD}{\rho_{soil}} - \Theta_{sw} \right]$$

Where:		Units
ksv	COPC loss constant due to volatilization	yr^{-1}
3.1536 x 10^7	units conversion factor	s/yr
H	Henry's Law constant; COPC-specific	atm-m^3/mol
Z_s	soil mixing zone depth; discussed previously	cm
KD_s	soil/water partition coefficient; COPC-specific	mL/mol
R	universal gas constant (8.205 x 10^{-5})	atm-m^3/mol-K
T_a	ambient air temperature	K
BD	soil bulk density (1.5 g/cm^3)	g soil/cm^3 soil
D_a	diffusivity of COPC in air	cm^2/s
ρ_{soil}	solids particle density (2.7 g/cm^3)	g/cm^3
θ_{sw}	soil volumetric water content (0.2 mL/cm^3)	mL/cm^3

The ambient air temperature (T_a) is equal to the annual average temperature (7.1°C).

1.3   Vegetation

Indirect exposure from the ingestion of homegrown produce depends on the total concentration of chemical in the leafy, fruit and root portions of the plant. Due to general differences in contaminant uptake, ingestion of produce is separated into two categories – above-ground and below ground produce. Above-ground produce is further subdivided into exposed and protected categories.

Chemical concentrations in above-ground exposed produce were calculated by taking the sum of contamination through direct deposition of particles (wet and dry), vapour transfer, and root uptake. Above-ground protected produce such as peas, beans, and corn are covered by a

protective coating and therefore are not exposed to direct deposition or vapour transfer. Root uptake is the primary mechanism of exposure for above-ground protected produce. As well, below ground produce is not exposed to direct deposition or vapour transfer and root uptake was the only pathway of exposure evaluated.

Concentrations in fruit and vegetables were calculated separately in the model. Fruit was considered to be exposed to the same contamination pathways as above-ground exposed produce. The difference was that the US EPA (2005) provides fruit and produce specific values for the calculation of contamination due to direct deposition.

Calculation of COPC concentration in traditional plants and wild fruit was also completed using the equations below.

1.3.1 Above-ground Produce Concentration Due to Direct Deposition

(13)

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

Where:		Units
Pd	plant (above-ground produce) concentration due to direct (wet and dry) deposition	mg COPC/kg DW
1,000	units conversion factor	mg/g
$Hg_{factorAG}$	mercury factor for above-ground plants; discussed below	unitless
Q	COPC emission rate; discussed previously	g/s
F_v	fraction of chemical air concentration in vapour phase; discussed previously	unitless
Dydp	Unitized yearly dry deposition from particle phase; discussed previously	s/m^2 yr^{-1}
Fw	fraction of chemical wet deposition that adheres to plant surfaces; discussed below	unitless
Dywp	Unitized yearly wet deposition from particle phase; discussed previously	s/m^2 yr^{-1}
Rp	interception fraction of the edible portion of the plant; discussed below	unitless
kp	plant surface loss coefficient; discussed below	yr^{-1}
Tp	length of plant exposure to deposition per harvest of the edible portion of the ith plant group; discussed below	yr
Yp	yield or standing crop biomass of the edible portion of the plant (productivity), discussed below	kg DW/m^2

The $Hg_{factorAG}$ for above-ground plants is 1.0 for all COPCs, with the following exceptions:
- for Hg^0 (i.e., 0.482 * 0.0)
- 0.37596 for Hg^{2+} (i.e., 482 * 0.78)
- 0.106044 for MHg (i.e., 0.482 * 0.22)

The Fw values adopted from US EPA (2005) were as follows; 0.2 for anions, 0.6 for cations and most organics.

The values of Fw, Rp, kt, Tp, and Yp are neither site nor COPC-specific. The values used in this assessment (from US EPA, 2005) differ for fruits, vegetables, silage, and forage, and are presented below.

Variable	Vegetable	Fruit	Silage	Forage
Rp	0.982	0.053	0.46	0.5
kp	18	18	18	18
Tp	0.164	0.164	0.16	0.12
Yp	5.66	0.252	0.8	0.325

1.3.2 Above-ground Produce Concentration Due to Air-to-Pant Transfer

The estimation of chemical concentrations in exposed above-ground produce from air-to-plant transfer considers the limitations of chemicals to transfer from plant surfaces to the inner portions of the plant.

(14)

$$Pv = \left[Q \times F_v \times Cyv \right] \times Bv_{ag} \times VG_{ag} \times \frac{Hg_{factor}}{\rho_a}$$

Where: Units

Pv	plant (above-ground produce) concentration due to air-to-plant transfer	μg COPC/g DW
Q	COPC emission rate; discussed previously	g/s
F_v	fraction of chemical air concentration in vapour phase; COPC-specific	unitless
Cyv	yearly average air concentration from vapour phase; discussed previously	μg/m^3
Bv_{ag}	air-to-plant biotransfer factor; COPC-specific ([mg COPC/g DW plant]/[mg COPC/g air])	unitless
VG_{ag}	empirical correction factor for above-ground produce; discussed below	unitless
$Hg_{factorAG}$	mercury factor for above-ground plants; discussed previously	unitless
ρ_a	density of air (1,200)	g/m^3

For forage and silage, the VG_{ag} factor is different. To use the above factors to estimate COPC concentrations specifically for forage and silage assumes that there is insignificant translocation of COPCs deposited on the surface of bulky silage to the inner parts of the vegetation. Forage and silage are considered vegetative plant parts, and grains are considered reproductive plant parts. US EPA (2005) recommends using VG_{ag} values of 1.0 for forage and 0.5 for silage. These values have been adopted in this assessment.

1.3.3 Produce Concentration Due to Root Uptake

Root uptake contributes to chemical concentrations in both above-ground and below ground produce. The US EPA (2005) has provided two separate equations to estimate chemical concentrations in the edible portions of above and below ground produce.

Above-ground produce (exposed and protected):

$$Pr = Cs \times Br_{ag} \qquad (15)$$

Below-ground produce:

$$Pr = \frac{Cs \times RCF \times VG_{rootveg}}{Kd_S \times 1 kg/L} \qquad (16)$$

Where:		Units
Pr	concentration of chemical in produce due to root uptake	mg/kg
Br_{ag}	plant-soil bioconcentration factor for above-ground produce; COPC-specific	unitless
$VG_{rootveg}$	empirical correction factor for belowground produce (0.01 or 1.0, see discussion above)	unitless
Kd_s	soil-water partition coefficient (K_{oc} x *foc*)	L/kg
Cs	average soil concentration over exposure duration (mg COPC/kg soil)	mg/kg
RCF	root concentration factor	unitless

The above-ground produce equation is based on the approach developed by Travis and Arms (1988). This equation is appropriate for estimating chemical concentrations in exposed and protected above-ground produce but not below ground produce. The equation for estimating concentrations in below ground produce includes a root concentration factor that was developed by Briggs et al. (1982). The root concentration factor is the ratio of chemical in the root to the chemical in the soil water.

The plant-soil bioconcentration factor (Br_{ag}) differed depending on the type of plant (vegetable, root vegetable (applicable only for metals), fruit, forage, or grain). In general, for all but the inorganics, the Br_{ag} for all plant types was the same, that is $Br_{ag(veg)} = Br_{ag(fruit)} = Br_{ag(forage)} = Br_{ag(grain)}$. For metals, a $Br_{rootveg}$ value was calculated by dividing RCF by Kd_s, Br_{ag} value was calculated using methodology and data from Baes, et al. (1984): The Br value for nonvegetative growth (reproductive) in Baes, et al. (1984) was used for $Br_{ag(fruit)}$. A Br value for nonvegetative (reproductive) growth and Bv values (equal to $Br_{ag(forage)}$) for vegetative growth weighted as 75% (reproductive) and 25% vegetative were used for $Br_{ag(veg)}$. The Br_{ag} was calculated as a weighted average of (1) $Br_{ag(fruit)}$ combined with a human consumption rate of fruits of 1.44×10^{-03} kg/kg/day, and (2) $Br_{ag(veg)}$ combined with a human consumption rate of vegetables of 1.49×10^{-03} kg/kg/day. $Br_{ag(grain)}$ is equal to $Br_{ag(fruit)}$. All Br_{ag} values for elemental mercury were set to zero, as it is assumed that elemental mercury does not deposit onto soils; therefore, there would be no plant uptake through the soil.

1.4   Animal Tissue

Chemical concentrations in an animal are estimated on the basis of the amount of chemical that the animal is assumed to consume through their diet. Additional contamination may occur through the incidental ingestion of soil.

The total concentration of chemicals in forage is calculated using the same formulae as were used for the homegrown produce estimates. Forage is assumed to be above-ground exposed

produce. US EPA (2005) recommends that 100 percent of plant material eaten by wild game is assumed to have been grown on soil contaminated by emission sources.

US EPA (2005) recommends using the equation presented in 1.3.1 to calculate forage concentrations due to direct deposition. As previously discussed, the recommended value for Rp (interception fraction of the edible portion of the plant) for forage is 0.5, the recommended value for Tp (plant exposure length to deposition per harvest of the edible portion of the plant) for forage is 0.12, while the recommended value of Tp (standing crop biomass (productivity)) for forage is .24 kg DW/m^2. In addition, the recommended value for VG_{ag} (empirical correction factor) for forage is 1.0.

1.4.1 Beef

The following equation calculates the COPC concentration in beef through the ingestion of contaminated plants and soil.

(17)

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

Where:		Units
A_{Beef}	Concentration of COPC in Beef	mg COPC/kg
F_i	Fraction of plant type i grown on contaminated soil and ingested by the animal	unitless
Qp_i	Quantity of plant type i eaten by the animal each day	kg DW plant/day
P_i	Concentration of COPC in plant type i eaten by the animal	mg/kg DW
Qs	Quantity of soil eaten by the animal each day	kg soil/day
Cs	Average soil concentration over exposure duration	mg COPC/kg soil
Bs	Soil bioavailability factor	unitless
Ba_{Beef}	COPC biotransfer factor	day/kg WW tissue
MF	Metabolism Factor	unitless

1.4.2 Milk

The following equation calculates the COPC concentration in milk through the ingestion of contaminated plants and soil.

(18)

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

Where: Units

Appendix C – Predictive Assessment Methods

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

1.4.3   Pork

The following equation calculates the COPC concentration in pork through the ingestion of contaminated plants and soil.

(19)

$$A_{Pork} = \left(\sum (F_i \; x \; Qp_i \; x \; P_i) + Qs \; x \; Cs \; x \; Bs \right) x \; Ba_{Pork} \; x \; MF$$

Where:		Units
A_{Pork}	Concentration of COPC in Pork	mg COPC/kg
F_i	Fraction of plant type i grown on contaminated soil and ingested by the animal	unitless
Qp_i	Quantity of plant type i eaten by the animal each day	kg DW plant/day
P_i	Concentration of COPC in plant type i eaten by the animal	mg/kg DW
Qs	Quantity of soil eaten by the animal each day	kg soil/day
Cs	Average soil concentration over exposure duration	mg COPC/kg soil
Bs	Soil bioavailability factor	unitless
Ba_{Pork}	COPC biotransfer factor	day/kg WW tissue
MF	Metabolism Factor	unitless

1.4.4   Chicken or Eggs

The following equation calculates the COPC concentration in chicken or eggs through the ingestion of contaminated plants and soil.

(20)

$$A_{Chicken} \text{ or } A_{Egg} = \left(\sum (F_i \times Qp_i \times P_i) + Qs \times Cs \times Bs \right) \times \left(Ba_{Chicken} \text{ or } Ba_{Egg} \right)$$

Where:		Units
$A_{Chicken\ or\ Egg}$	Concentration of COPC in Chicken or Egg	mg COPC/kg
F_i	Fraction of plant type i grown on contaminated soil and ingested by the animal	unitless
Qp_i	Quantity of plant type i eaten by the animal each day	kg DW plant/day
P_i	Concentration of COPC in plant type i eaten by the animal	mg/kg DW
Qs	Quantity of soil eaten by the animal each day	kg soil/day
Cs	Average soil concentration over exposure duration	mg COPC/kg soil
Bs	Soil bioavailability factor	unitless
$Ba_{Chicken\ or\ Egg}$	COPC biotransfer factor	day/kg WW tissue

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1.4.5 Wild Game

The following equation calculates the COPC concentration in wild game through the ingestion of contaminated plants and soil. The diet of wild game is assumed to consist of forage. The equation includes a biotransfer and metabolism factors to transform the daily animal intake of a COPC into an animal COPC tissue concentration (mg COPC/kg tissue).

(21)

$$C_{wildgame} = F_{forage} \times Qp_{forage} \times P_{forage} + Q_s \times C_s \times B_s + Q_w \times C_{wtot} \times Ba_{wildgame} \times MF$$

Where:		Units
C_{game}	concentration of chemical in wild game	mg/kg FW
F_{forage}	fraction of forage grown on contaminated soil and ingested by wild game (1.0)	unitless
Qp_{forage}	quantity of forage eaten by wild game per day; discussed below	kg DW/day
P_{forage}	concentration of chemical in forage eaten by wild game	mg/kg DW
Q_s	quantity of soil eaten by wild game each day	kg/day
C_s	average soil concentration over exposure duration; see section A.4.4.1.1	mg/kg
B_s	soil bioavailability factor	unitless
Ba_{game}	chemical-specific biotransfer factor for wild game	day/kg FW
Q_w	quantity of water consumed by wild game per day	L/day
C_{wtot}	total COPC concentration in the water column	mg/L
MF	metabolism factor	unitless

The quantity of forage eaten by wild game per day (Qp_{forage}) was estimated to be 1.72 kg DW plant/day.

The COPC-specific biotransfer factors for wild game (Ba_{game}) were calculated as follows:

$$Ba_{game} = Ba_{beef} \times \frac{0.10}{0.19} \tag{21}$$

Where 0.10 (10%) is the assumed fat content of game and 0.19 (19%) is the assumed fat content of beef.

Ba_{beef} is calculated as follows:

$$Ba_{beef} = 10^{logBa_{fat}} \times 0.19 \tag{22}$$

Where Ba_{fat} is calculated as follows:

$$logBa_{fat} = -0.099 \; logK_{ow}^{\;2} + 1.07logK_{ow} - 3.56 \tag{23}$$

The above equation is only suitable for K_{ow} values between -0.67 and 8.2. Where K_{ow} values fell above or below this range, the K_{ow} was assigned the cap values at the high or low end of the range; respectively.

The metabolism factor (MF) estimates the amount of COPC that remains in fat and muscle. Based on a study by Ikeda et al. (1980), US EPA (1995) used a COPC-specific MF to account for metabolism in animals and humans. Evidence indicates that bis(2-ethylexyl)phthalate (BEHP) is more readily metabolized and excreted by mammalian species than other contaminants (ATSDR, 1987), therefore, US EPA (2005) recommends a MF of 0.01 for BEHP. Lacking data to support derivation of other chemical-specific MFs, they recommend using a MF of 1.0 for all COPCs other than BEHP. A value of 1.0 has been adopted for all COPCs in this assessment, with the exception of polycyclic aromatic hydrocarbons, which have been assigned a MF of 0.01 based on a study (Hoefelt, 2001) that showed a 1,000 fold decrease in the retention of PAHs with respect to other chemicals. A 10% factor of safety was applied, resulting in a MF of 0.01 for all PAHs.

1.5   Drinking Water and Fish Tissue

The model calculates COPC concentrations in surface water for all waterbodies that were selected for evaluation. Calculations for rivers and lakes (surface waterbodies) are completed separately. Chemical loading to the water column was calculated through direct deposition, runoff from pervious and impervious surfaces in the watershed, soil erosion, direct diffusion of vapour phase COPCs into surface water, and internal transformation of compounds chemically or biologically. Consideration of other potential mechanisms may be appropriate, due to site-specific conditions (e.g., tidal influences); however, it is typically assumed that contributions from other potential mechanisms are negligible compared to those evaluated below.

1.5.1   Total COPC Load to Waterbody

The total COPC load to the Waterbody by all mechanisms discussed above is calculated as follows (US EPA, 2005):

$$L_T = L_{DEP} + L_{dif} + L_{RI} + L_R + L_E + L_I \tag{24}$$

Where: Units

L_T	total COPC load to the waterbody (including deposition, runoff, and erosion	g/yr
L_{DEP}	total (wet and dry) particle phase and vapour phase COPC direct deposition load to waterbody; discussed below	g/yr
L_{dif}	vapour phase COPC diffusion load to waterbody; discussed below	g/yr
L_{RI}	runoff load from impervious surfaces; discussed below	g/yr
L_R	runoff load from pervious surfaces; discussed below	g/yr
L_E	soil erosion load; discussed below	g/yr
L_I	internal transfer; (0) discussed below	g/yr

Due to the limited data and uncertainty associated with the chemical or biological internal transfer, L_I, of compounds into degradation products, US EPA (2005) generally recommends that a default value for this variable of zero be adopted. A value of zero has been adopted for this assessment.

1.5.2 Total Particle and Vapour Phase Direct Deposition Load to Waterbody

$$L_{DEP} = Hg_{factorWL} \times Q \times \left[F_v \times Dytwv + \left(1 - F_v \right) \times Dytwp \right] \times A_w \tag{25}$$

Where: Units

L_{DEP}	total (wet and dry) particle phase and vapour phase COPC direct deposition load to waterbody	g/yr
$Hg_{factorWL}$	mercury factor for water loading; discussed below	unitless
Q	COPC emission rate; discussed previously	g/s
F_v	fraction of COPC air concentration in vapour phase; discussed previously	unitless
Dytwv	yearly (waterbody or watershed) average total (wet and dry) deposition from vapour phase; discussed below	g/m^2-yr
Dytwp	yearly (waterbody or watershed) average total (wet and dry) deposition from particle phase; discussed below	g/m^2-yr
A_w	waterbody surface area	m^2

The $Hg_{factorWL}$ for water loading is 1.0 for all COPCs, with the following exceptions:
- 0.00 for Hg0
- 0.482 for Hg^{2+}
- 0.00 for MHg

The deposition terms (Dytwv and Dytwp) are a result of the air modelling. The area of the waterbody was assumed to be one square kilometre.

1.5.3 Vapour Phase COPC Diffusion Load to Waterbody

(26)

$$L_{dif} = \frac{K_v \times Hg_{factorWL} \times Q \times F_v \times Cywv \times A_w \times 1 \times 10^{-6}}{\dfrac{H}{R \times T_{wk}}}$$

Where:		Units
L_{dif}	vapour phase COPC diffusion load to waterbody	g/yr
K_v	overall COPC transfer rate coefficient; discussed below	m/yr
$Hg_{factorWL}$	mercury factor for water loading; discussed previously	unitless
Q	COPC emission rate; discussed previously	g/s
F_v	fraction of COPC air concentration in vapour phase; discussed previously	unitless
Cywv	yearly (waterbody or watershed) average air concentration from vapour phase discussed previously	$\mu g/m^3$
A_w	waterbody surface area; discussed previously	m^2
10^{-6}	units conversion factor	$g/\mu g$
H	Henry's Law constant; COPC-specific	atm-m^3/mol
R	Universal gas constant (8.205 x 10^{-5})	atm-m^3/mol-K
T_{wk}	waterbody temperature, waterbody-specific	K

The overall COPC transfer rate coefficient (K_v) was calculated using the following equation:

(27)

$$K_V = \left[K_L^{-1} + \left(K_G \times \frac{H}{RT_{wk}} \right)^{-1} \right]^{-1} \times \theta^{T_{wk} - 293}$$

Where:		Units
K_v	overall COPC transfer rate coefficient	m/yr
K_L	liquid phase transfer coefficient; discussed below	m/yr
K_G	gas phase liquid transfer coefficient; discussed below	m/yr
H	Henry's Law constant; COPC-specific	atm-m^3/mol
R	Universal gas constant (8.205 x 10^{-5} at 20°C)	atm-m^3/mol-K
T_{wk}	waterbody temperature	K
θ	temperature correction factor (1.026)	unitless

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. The value of the conductivity K_v depends on

the intensity of turbulence in the waterbody and the overlying atmosphere. This equation assumes that volatilization occurs much less readily in lakes and reservoirs than in moving waterbodies.

The liquid phase transfer coefficient (K_L) is calculated differently, depending on the body of water, as detailed below:

For flowing streams or rivers (transfer coefficient controlled by flow-induced turbulence):

$$K_L = \sqrt{\frac{1 \times 10^{-4} \times D_w \times u}{d_z} \times 3.1536 \times 10^7} \tag{28}$$

For quiescent lakes or ponds (transfer coefficient controlled by wind-induced turbulence):

$$K_L = C_d^{0.5} \times W \times \left(\frac{\rho_a}{\rho w}\right)^{0.5} \times \frac{k^{0.33}}{\lambda_z} \times \left(\frac{\mu_w}{\rho_w \times D_w}\right)^{-0.67} \times 3.1526 \times 10^7 \tag{29}$$

Where:		Units
K_L	liquid phase transfer coefficient	m/yr
D_w	diffusivity of COPC in water; COPC-specific	cm^2/s
μ	current velocity; waterbody specific	m/s
1×10^{-4}	units conversion factor	m^2/cm^2
d_z	total waterbody depth; waterbody specific	m
C_d	drag coefficient (0.0011)	unitless
W	average annual wind speed (1.4)	m/s
ρ_a	density of air (0.0012 at standard conditions)	g/cm^3
ρ_w	density of water (1)	g/cm^3
k	von Karman's constant (0.4)	unitless
λ_z	dimensionless viscous sublayer thickness (4)	unitless
μ_w	viscosity of water corresponding to water temperature (0.0169)	g/cm-s
3.1536×10^7	units conversion factor	s/yr

The following equation is recommended (US EPA, 2005) to calculate the gas phase transfer coefficient:

For quiescent lakes or ponds:

$$K_G = C_d^{0.5} \times W \times \frac{k^{0.33}}{\lambda_z} \times \left(\frac{\mu_a}{\rho_a \times D_a}\right)^{-0.67} \times 3.1536 \times 10^7 \tag{30}$$

Where:	Units

K_G	gas phase transfer coefficient	m/yr
C_d	drag coefficient; discussed previously	unitless
W	average annual wind speed	m/s
k	von Karman's constant; discussed previously	unitless
λ_z	dimensionless viscous sublayer thickness; discussed previously	unitless
μ_a	viscosity of air corresponding to water temperature (1.81×10^{-4})	g/cm-s
ρ_a	density of air; discussed previously	g/cm^3
D_a	diffusivity of COPC in air; COPC-specific	cm^2/s
3.1536×10^7	units conversion factor	s/yr

For flowing streams or rivers, US EPA (2005) recommends using a value of K_G = 36,500 m/yr., because the rate of transfer of COPC from the gas phase for a flowing stream or river is assumed to be constant.

(31)

$$L_{RI} = Hg_{factorWL} \times Q \times \left[F_v \times Dytwv + \left(1.0 - F_v \right) \times Dytwp \right] \times A_I$$

1.5.4 Runoff Load from Impervious Surfaces

Where:		Units
L_{RI}	runoff load from impervious surfaces	g/yr
$Hg_{factorWL}$	mercury factor for water loading; discussed previously	unitless
Q	COPC emission rate; discussed previously	g/s
F_v	fraction of COPC air concentration in vapour phase; discussed previously	unitless
Dytwv	yearly (waterbody or watershed) average total (wet and dry) deposition from vapour phase; discussed previously	g/m^2-yr
Dytwp	yearly (waterbody or watershed) average total (wet and dry) deposition from particle phase; discussed previously	g/m^2-yr
A_I	impervious watershed area receiving COPC deposition	m^2

The 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 waterbody. This value is watershed-specific.

1.5.5 Runoff Load from Pervious Surfaces

(32)

$$L_R = RO \times \left(A_L - A_I \right) \times \frac{Cs \times BD}{\theta_{sw} + Kd_s \times BD} \times 0.01 \times Hg_{factorRL}$$

Appendix C – Predictive Assessment Methods

Where: <u>Units</u>

L_R	runoff load from pervious surfaces	g/yr
RO	average annual surface runoff from pervious areas; discussed previously	cm/yr
A_L	total watershed area receiving COPC deposition; waterbody-specific	m^2
A_I	impervious watershed area receiving COPC deposition; waterbody specific	m^2
Cs	average soil concentration over exposure duration (in watershed soils)	mg COPC/kg soil
BD	soil bulk density (1.5 g/cm^3)	g soil/cm^3 soil
θ_{sw}	soil volumetric water content (0.2 mL/cm^3)	mL water/cm^3 soil
Kd_s	soil-water partition coefficient, COPC-specific	cm^3 water/g soil
0.01	units conversion factor	kg-cm^2/mg-m^2

1.5.6   Soil Erosion Load

(33)

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

Where: <u>Units</u>

L_E	soil erosion load	g/yr
X_e	unit soil loss; discussed previously	kg/m^2-yr
A_L	total watershed area receiving COPC deposition; previously discussed	m^2
A_I	impervious watershed area receiving COPC deposition; previously discussed	m^2
SD	sediment delivery ratio (watershed); discussed previously	unitless
ER	soil enrichment ratio; discussed previously	unitless
Cs	average soil concentration over exposure duration (in watershed soils)	mg COPC/kg soil
BD	soil bulk density (1.5 g/cm^3)	g soil/cm^3 soil
θ_{sw}	soil volumetric water content (0.2 mL/cm^3)	mL water/cm^3 soil
Kd_s	soil-water partition coefficient; COPC-specific	cm^3 water/g soil
0.001	units conversion factor	k-cm^2/mg-m^2

1.5.7   Drinking Water Concentration

US EPA recommends using the following equation to calculate the total waterbody COPC concentration, which includes both the water column and the bed sediment.

To be conservative it was assumed that receptors would consume water directly from the water column of the waterbody without any prior filtering.

(34)

$$C_{wtot} = \frac{L_T}{Vf_x \times f_{wc} + k_{wt} \times A_W \times d_{wc} + d_{bs}}$$

Where: Units

C_{wtot}	total waterbody COPC concentration (including water column and bed sediment)	g COPC/m^3 waterbody
L_T	total COPC load to the waterbody (including deposition, runoff, and erosion); presented previously	g/yr
Vf_x	average volumetric flow rate through waterbody; discussed below	m^3/yr
f_{wc}	fraction of total waterbody COPC concentration in the water column; discussed below	unitless
k_{wt}	overall total waterbody COPC dissipation rate constant; discussed below	yr^{-1}
A_W	waterbody surface area; waterbody-specific	m^2
d_{wc}	depth of water column; waterbody-specific	m
d_{bs}	depth of upper benthic sediment layer (0.03m)	m

The average volumetric flow rate through the waterbody (Vf_x) was calculated using the water balance model equation if data was available, otherwise, average volumetric flow rate was estimated for the lake based on the equation presented in US EPA (2005) [Watershed Area x (1/2) average annual RO].

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, the US EPA (2005) recommends values from 0.01 to 0.05 and a default value of 0.03, which represents the midpoint of the specified range. This value has been adopted for use in this assessment.

US EPA (2005) recommends using the following equation to calculate f_{wc} (the fraction of total waterbody COPC concentration in the water column). In addition, the equation for f_{bs} is presented.

(35)

$$f_{wc} = \frac{1 + Kd_{sw} \times TSS \times 1 \times 10^{-6} \times d_{wc}/d_z}{1 + Kd_{sw} \times TSS \times 1 \times 10^{-6} \times d_{wc}/d_z + \theta_{bs} + Kd_{bs} \times C_{BS} \times d_{bs}/d_z}$$

Where: Units

f_{wc}	fraction of total waterbody COPC concentration in the water column	unitless
f_{bs}	fraction of total waterbody COPC concentration in benthic sediment	unitless
Kd_{sw}	suspended sediments/surface water partition coefficient; COPC-specific	L water/kg suspended sediment
TSS	total suspended solids concentrations; discussed below	mg/L
1×10^{-6}	units conversion factor	kg/mg

Appendix C – Predictive Assessment Methods

d_z	total waterbody depth; discussed below	m
θ_{bs}	bed sediment porosity; discussed below	$L_{water}/L_{sediment}$
Kd_{bs}	bed sediment/sediment pore water partition coefficient; COPC-specific	L water/kg bottom sediment
C_{BS}	bed sediment concentration; discussed below	g/cm^3 [equivalent to kg/L]
d_{wc}	depth of water column; water-body specific	m
dbs	depth of upper benthic sediment layer; discussed previously	m

The total waterbody depth (d_z) is calculated by adding the depth of the water column to the depth of the upper benthic layer ($d_{wc}+d_{bs}$).

US EPA (2005) recommends using waterbody-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. If measured data are not available, or of unacceptable quality, US EPA (2005) recommends the following equation be used to calculate the TSS for non-flowing bodies of water:

(36)

$$TSS = \frac{X_e \times \left(A_L - A_I \right) \times SD \times 1 \times 10^3}{Vf_x + D_{ss} \times A_W}$$

Where:		Units
TSS	total suspended solids concentration	mg/L
X_e	unit soil loss; discussed previously	kg/m^2-yr
A_L	total watershed area (evaluated) receiving COPC deposition; discussed previously	m^2
A_I	impervious watershed area receiving COPC deposition; discussed previously	m^2
SD	sediment delivery ratio (watershed); discussed previously	unitless
1×10^3	units conversion factor	
Vf_x	average volumetric flow rate through waterbody; discussed previously	m^3/yr
D_{ss}	suspended solids deposition rate (1,825)	m/yr
A_W	waterbody surface area	m^2

For the purpose of this assessment, TSS values were calculated.

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.

US EPA (2005) recommends the following default values (which have been adopted for bed sediment porosity (θ_{bs}), adapted from NC DEHNR (1997):

$$\theta_{bs} = 0.6 \ L_{water}/L_{sediment}$$
Assuming:
$$\rho_s = 2.65 \ kg/L \ [bed \ sediment \ density]$$
And:
$$C_{BS} = 1.0 \ kg/L \ [bed \ sediment \ concentration]$$

US EPA (2005) recommends the following equation to calculate the overall dissipation rate of COPCs in surface water, resulting from volatilization and benthic burial:

(37)

$$k_{wt} = f_{wc} \times k_v + f_{bs} \times k_b$$

Where: Units

k_{wt}	overall total waterbody dissipation rate constant	yr^{-1}
f_{wc}	fraction of total waterbody COPC concentration in the water column; discussed above	unitless
k_v	water column volatilization rate constant	yr^{-1}
f_{bs}	fraction of total waterbody COPC concentration in benthic sediment; discussed above	unitless
k_b	benthic burial rate constant; discussed below	yr^{-1}

The water column volatilization rate constant (k_v) is calculated as follows:

(38)

$$k_v = \frac{K_v}{d_z \times \left(1 + Kd_{sw} \times TSS \times 1 \times 10^{-6}\right)}$$

Where: Units

k_v	water column volatilization rate constant	yr^{-1}
K_v	overall COPC transfer rate coefficient; discussed previously	m/yr
d_z	total waterbody depth; discussed previously	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 recommended equation (US EPA. 2005) for benthic burial rate constant (k_b) is presented below:

(39)

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

Where: Units

k_b	benthic burial rate constant	yr^{-1}
X_e	unit soil loss; discussed previously	kg/m^2-yr
A_L	total watershed area (evaluated) receiving deposition; discussed previously	m^2

Appendix C – Predictive Assessment Methods

SD	sediment delivery ratio (watershed); discussed previously	unitless
Vf_x	average volumetric flow rate through waterbody; discussed previously	m^3/yr
TSS	total suspended solids concentration; discussed previously	mg/L
A_W	waterbody surface area; waterbody-specific	m^2
C_{BS}	bed sediment concentration; discussed previously	g/cm^3
d_{bs}	depth of upper benthic sediment layer; discussed previously	m
$1x10^{-6}$	units conversion factor	kg/mg
$1x10^3$	units conversion factor	g/kg

The US EPA (2005) recommends using the following equation to calculate the total COPC concentration in the water column (C_{wctot}):

(40)

$$C_{wctot} = f_{wc} \times C_{wtot} \times \frac{d_{wc} + d_{bs}}{d_{wc}}$$

Where: Units

C_{wctot}	total COPC concentration in water column; discussed previously	mg COPC/L water column
f_{wc}	fraction of total waterbody COPC concentration in the water column; discussed previously	unitless
C_{wtot}	total waterbody COPC concentration, including water column and bed sediment; discussed previously	mg COPC/L waterbody
d_{wc}	depth of water column; discussed previously	m
d_{bs}	depth of upper benthic sediment layer; discussed previously	m

The recommended equation for calculating the concentration of COPC dissolved in the water column (C_{dw}) is as follows (US EPA, 2005):

(41)

$$C_{dw} = \frac{C_{wctot}}{1 + Kd_{sw} \times TSS \times 1 \times 10^{-6}} \times Hg_{factorC_{dw}}$$

Where: Units

C_{dw}	dissolved phase water concentration	mg COPC/L water
C_{wctot}	total COPC concentration in water column; discussed previously	mg COPC/L water column
Kd_{sw}	suspended sediments/surface water partition coefficient; COPC-specific	L water/kg suspended sediment
TSS	total suspended solids; discussed previously	mg/L
$1x10^{-6}$	units conversion factor	kg/mg
$Hg_{factorCdw}$	mercury factor for dissolved water concentration; discussed below	unitless

The $Hg_{factorCdw}$ for dissolved water concentration is 1.0 for all COPCs, with the following exceptions:

- 0.968 for Hg^{2+} (96.8% is the ratio of Inorganic Mercury (Hg^{+2}) to Total Mercury)
- 0.032 for MHg (3.2% is the ratio of Methyl Mercury (MHg) to Total Mercury)

The following equation is recommended for the calculation of COPC concentration sorbed to bed sediment (C_{sb}):

(42)

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

Where:

		Units
C_{sb}	COPC concentration sorbed to bed sediment	mg COPC/kg sediment
f_{bs}	fraction of total waterbody COPC concentration in benthic sediment; discussed previously	unitless
C_{wtot}	total waterbody COPC concentration, including water column and bed sediment; discussed previously	mg COPC/L waterbody
Kd_{bs}	bed sediment/sediment pore water partition coefficient; COPC-specific	L COPC/kg waterbody
θ_{bs}	bed sediment porosity; discussed previously	$L_{pore\ water}/L_{sediment}$
C_{BS}	bed sediment concentration; discussed previously	g/cm^3
d_{wc}	depth of water column; discussed previously	m
d_{bs}	depth of upper benthic sediment layer; discussed previously	m

1.5.8   Fish Concentrations

Chemical concentrations in fish were calculated using either a COPC-specific bioconcentration factor (BCF), bioaccumulation factor (BAF), or biota-sediment accumulation factor (BSAF). In accordance with US EPA (2005) guidance, extremely hydrophobic chemicals such as dioxins, furans, and PCBs are assumed to have a high tendency to bioaccumulate in bed sediments and therefore a BSAF was used to assess fish uptake for these chemicals. All other COPC were evaluated using BCF/BAFs.

Bioconcentration is the process by which a COPC is absorbed by a fish or aquatic organism only through its respiratory and dermal surfaces, dietary exposure is not included in this factor (Arnot & Gobas, 2006). The degree to which bioconcentration occurs in fish or aquatic organisms is expressed as the bioconcentration factor (BCF) (Arnot &Gobas, 2006). Bioaccumulation is the process by which a COPC is absorbed by a fish or aquatic organism via all routes of exposure including environmental exposure and dietary exposure (Arnot & Gobas, 2006). The BCFs and BAFs are generally based on dissolved water concentrations. Therefore, it's appropriate to calculate the COPC concentration in fish using dissolved water concentrations. The BSAF is the ratio of a COPC concentration in fish or an aquatic organism to the concentration of COPC in the sediment (Arnot &Gobas, 2006). The BSAF values are based on benthic sediment concentrations; therefore, when using BSAF values, US EPA (2005) recommend calculating COPC concentrations in fish using benthic sediment concentrations. The appropriate equations are presented below:

Fish Concentration Using BCF's or BAF's

(43)

$$C_{fish} = Hg_{factorFC} \times C_{dw} \times BCF_{fish} \text{ or } BAF_{fish} \times MF$$

Where: Units

C_{fish}	concentration of chemical in fish	mg CoPC/kg FW tissue
$Hg_{factorFC}$	mercury factor for fish concentration; discussed below	unitless
C_{dw}	concentration in water dissolved phase; previously discussed	mg CoPC/L
BCF_{fish}	chemical specific bioconcentration factor for fish; CoPC-specific	L/kg FW tissue
BAF_{fish}	chemical specific bioaccumulation factor for fish; CoPC-specific	L/kg FW tissue
MF	metabolism factor; discussed previously in Section 1.4.5	unitless

The $Hg_{factorFC}$ is 1.0 for all CoPCs, with the following exceptions:
- 0.0 for elemental mercury (Hg^0)
- 0.0 for divalent mercury (Hg^{2+})
- 1.0 for MHg

Fish Concentration Using BSAFs

(44)

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

Where: Units

C_{fish}	concentration of chemical in fish	mg CoPC/kg FW tissue
C_{sb}	concentration sorbed to bed sediment; previously discussed	mg CoPC/kg bed sediment
f_{lipid}	fish lipid content; site-specific and dependent on type of fish consumed	unitless
BSAF	CoPC-specific biota-to-sediment accumulation factor	sediments/kg fish FW
OC_{sed}	fraction of organic carbon in bottom sediment; discussed below	unitless
MF	metabolism factor; discussed previously in Section 1.4.1	unitless

The fraction of organic carbon in bottom sediment (OC_{sed}) is waterbody specific. A value of 0.05 was assumed for the lake. The US EPA (2005) default is 0.04; however, values can range between 0.01 and 0.25.

Mercury Modelling

The US EPA HHRAP constitutes a series of numerical models designed to estimate the environmental fate, transport, and uptake of airborne contaminants. Each model includes default assumptions and, like any other generic guidance, is constructed in a conservative manner. In the case of mercury modelling, the HHRAP includes a series of conservative default

assumptions that multiply together to lead to predictions that are higher than could reasonably be expected and that are often in disagreement with empirical data (Zemba et al., 2001).

Speciation of Mercury Emissions

The US EPA HHRAP is a risk assessment protocol designed specifically for the evaluation of hazardous waste combustion facilities. However, it's use has been commonly extrapolated to assess other situations. Stack emissions are speciated into both divalent (Hg^{2+}) and elemental (Hg^0) mercury, and include both vapour and particle-bound forms. Divalent mercury emitted either in the vapour phase or particle-bound is subject to much faster atmospheric removal than elemental mercury (Lindberg et al., 1992; Peterson et al., 1995; Shannon and Volder, 1994) and therefore has a much more significant impact on near-field deposition. The vast majority of elemental mercury dissipates into the global mercury cycle.

Percentages of Hg^{2+} and Hg^0, vapour and particle-bound, vary widely depending on the source. The HHRAP made the following default assumptions for the phase allocation and speciation of mercury in air:
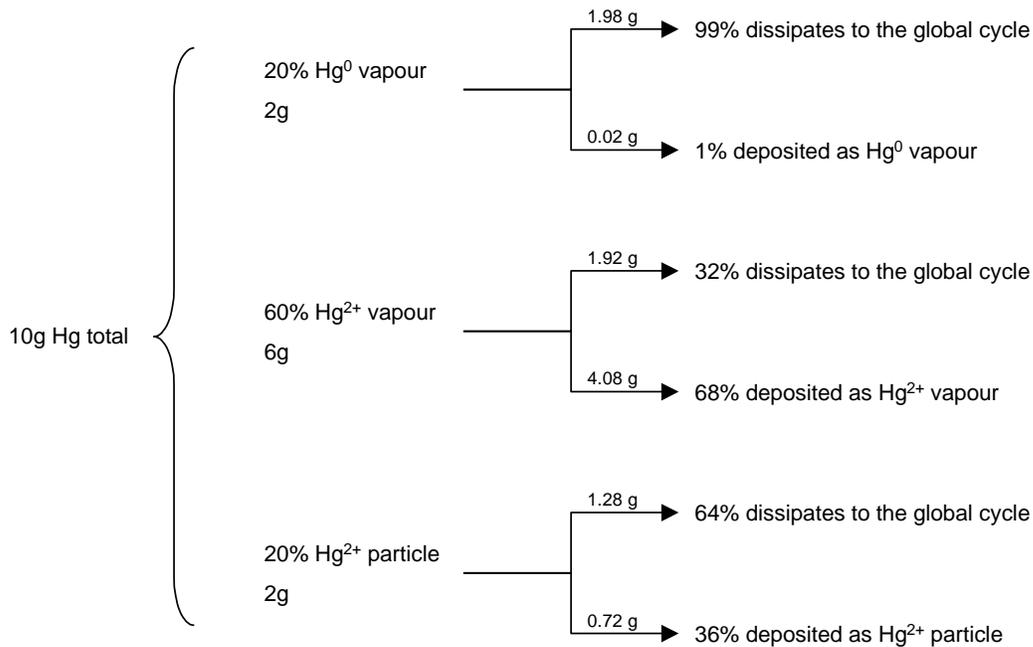
1-1 Phase Allocation and Speciation of Mercury Emissions - US EPA HHRAP Default Assumptions

Based on the above, 48.2% (0.02g + 4.08g + 0.72g) of mercury emissions are assumed to deposit locally. This default allocation in the HHRAP is based on the following:

- Consistency with emissions speciation data for hazardous waste combustion sources; and

- High degree of protection, since it results in the highest percentage of total mercury being deposited near the source and, therefore, is indicative of the maximum risk.

The phase allocation in the HHRAP is based on data for municipal waste incinerators presented in the Mercury Report to Congress (US EPA, 1997b).

Mercury Methylation in Waterbodies

The great majority of mercury deposited on land is assumed to be inorganic. A portion of the total mercury deposited into a waterbody is then assumed to be converted into the organic form – methyl mercury – in the water. The HHRAP recommends a default methylation of mercury in the waterbody of 15% methyl mercury and 85% inorganic mercury. Both forms of mercury are accumulated into fish at different rates and then all of the fish tissue mercury is assumed to be converted to methyl mercury in the fish.

The 15% portion of total dissolved mercury that is assumed to be present as methyl mercury references the Report to Congress. In fact, a range of studies is referenced in the Report to Congress (Volume 3, Appendix D) which provide a range of methyl mercury fractions. The default value adopted in the HHRAP of 15% is the single maximum value from any of the quoted studies and is likely to overestimate the rate of methylation. The range of values presented from the other studies is from 4.6% up to 9.2% methyl mercury in the water. The point estimate for %methyl mercury given in the Report to Congress is 7.8%. This value is the median of all the studies presented.

Subsequently, the US EPA published the Water Quality Criterion for the Protection of Human Health: Methylmercury Final (US EPA, 2001). This criteria document provides discussion of mercury methylation in waterbodies and provides the following methyl mercury fractions:

- Lakes - 3.2%
- Rivers - 1.4%

2.0 REFERENCES

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