Mercury Fate and Transport: Example Calculation

Constants used in this calculation

Air Model Parameters

Cywv_wb := 0.04916806	Cywv := 0.06139385	Dywv := 0.0055	Chv := 10.26313	Cyp_pb := 0.06421
Dywwv_wb := 0.00324014	Dywwv := 0.00437744	Dydp_pb := 0.00594	Chp := 10.0224	
Dytwp_wb_pb := 0.00716708	Dytwp_pb := 0.00982131	Dywp_pb := 0.00312	Cyv := 0.06615	

Watershed and Water Body Parameters

USLEK := 0.36	USLEC := 0.5	USLEPF := 1	AL := 5946384	Aw := 731328.097
USLELS := 1.5	USLERF := 100	Cd := 0.0011	AI := $2.9731932 \cdot 10^{5}$	A := 1
Vfx := 0	k := 0.4	dbs := 0.03	dz := 1.03	

Exposure Scenario-Specific Parameters

BWadult := 70	Ffish := 1

Mercury-Specific Fate and Transport Parameters

DaHg2 := $4.531 \cdot 10^{-2}$	KdbsHg2 := 50000	DwHg2 := $5.2467 \cdot 10^{-6}$	KdsHg2 := 58000	Fdw := 1
DaMhg := $5.2777 \cdot 10^{-2}$	KdbsMhg := 3000	DwMhg := $6.1111 \cdot 10^{-6}$	KdsMhg := 7000	Ps := 2.7
Kdsw := $1 \cdot 10^{5}$	HHg2 := $7.1 \cdot 10^{-10}$	BAFfishMhg := $6.8 \cdot 10^{6}$	CRfish := 0.00117	ksg := 0
Fv := 0.85	HMhg := $4.7 \cdot 10^{-7}$	BAFfishHg2 := 0	RfD := $1 \cdot 10^{-4}$	
BVag := 1800	VGag := 1	VGrv := 1	CRdwadult := 1.4	

Mercury-Site-Specific Parameters

ERi := 1	ERo := 3	Fw := 0.6

Site-Specific Parameters

Cbs := 1	R := $8.205 \cdot 10^{-5}$	Θbs := 0.6	λz := 4	Ta := 298	Yp := 2.24
μw := $1.69 \cdot 10^{-2}$	P := 100	Θ := 1.026	a := 1.4	μa := $1.81 \cdot 10^{-4}$	Vdv := 3
ρw := 1	I := 100	Θsw := 0.2	b := 0.125	ρa := $1.2 \cdot 10^{-3}$	
Twk := 298	RO := 100	dwc := 1	Rp := 0.39	W := 1.0	
BD := 1.5	Ev := 100	kp := 18	Zs := 1	EF := 350	
ED := 30	tD := 100	Tp := 0.164	TSS := 10	AT := 30	

Source-Specific Emission Rate

Q := $2.1875 \cdot 10^{-5}$

Risk from Mercury Through the Fish Ingestion Pathway.

B-4-21 Gas Phase Transfer Coefficient - Quiescent lakes or ponds

$$KGHg2 := \left(Cd^{0.5}\cdot W\right)\cdot\frac{k^{0.33}}{\lambda z}\cdot\left(\frac{\mu a}{\rho a\cdot DaHg2}\right)^{-0.67}\cdot 3.1536\cdot 10^{7} \qquad KGHg2 = 86333.54351663143$$

$$KGMhg := \left(Cd^{0.5}\cdot W\right)\cdot\frac{k^{0.33}}{\lambda z}\cdot\left(\frac{\mu a}{\rho a\cdot DaMhg}\right)^{-0.67}\cdot 3.1536\cdot 10^{7} \qquad KGMhg = 95624.1293625658$$

B-4-13 Universal Soil Loss Equation

$$Xe := USLERF\cdot USLEK\cdot USLELS\cdot USLEC\cdot USLEPF\cdot\frac{907.18}{4047} \qquad Xe = 6.052349888806523$$

B-4-14 Sediment Delivery Ratio

$$SD := a\cdot AL^{-b} \qquad SD = 0.19922618411898$$

B-4-22 Benthic Burial Rate Constant

$$kb := \left(\frac{Xe\cdot AL\cdot SD\cdot 10^{3} - Vfx\cdot TSS}{Aw\cdot TSS}\right)\cdot\left(\frac{TSS\cdot 10^{-6}}{Cbs\cdot dbs}\right) \qquad kb = 0.326805894476895$$

B-4-16 Fraction in Water Column and Benthic Sediment

$$fwcHg2 := \frac{\left(1 + Kdsw\cdot TSS\cdot 10^{-6}\right)\cdot\frac{dwc}{dz}}{\left(1 + Kdsw\cdot TSS\cdot 1\cdot 10^{-6}\right)\cdot\frac{dwc}{dz} + (\Theta bs + KdbsHg2\cdot Cbs)\cdot\frac{dbs}{dz}} \qquad fwcHg2 = 0.001331541965542$$

$$fwcMhg := \frac{\left(1 + Kdsw\cdot TSS\cdot 10^{-6}\right)\cdot\frac{dwc}{dz}}{\left(1 + Kdsw\cdot TSS\cdot 1\cdot 10^{-6}\right)\cdot\frac{dwc}{dz} + (\Theta bs + KdbsMhg\cdot Cbs)\cdot\frac{dbs}{dz}} \qquad fwcMhg = 0.02173487795866$$

$fbsHg2 := 1 - fwcHg2$ $\quad fbsHg2 = 0.998668458034458$ $\quad fbsMhg := 1 - fwcMhg$ $\quad fbsMhg = 0.97826512204134$

B-4-20 Liquid Phase Transfer Coefficient - Quiescent lakes or ponds

$$KLHg2 := \left(Cd^{0.5}\cdot W\right)\cdot\left(\frac{\rho a}{\rho w}\right)^{0.5}\cdot\frac{k^{0.33}}{\lambda z}\cdot\left(\frac{\mu w}{\rho w\cdot DwHg2}\right)^{-0.67}\cdot 3.1536\cdot 10^{7} \qquad KLHg2 = 29.87810588409151$$

$$KLMhg := \left(Cd^{0.5}\cdot W\right)\cdot\left(\frac{\rho a}{\rho w}\right)^{0.5}\cdot\frac{k^{0.33}}{\lambda z}\cdot\left(\frac{\mu w}{\rho w\cdot DwMhg}\right)^{-0.67}\cdot 3.1536\cdot 10^{7} \qquad KLMhg = 33.09247716434865$$

B-4-19 Overall COPC Transfer Rate Coefficient

$$KVHg2 := \left[KLHg2^{-1} + \left(KGHg2 \cdot \frac{HHg2}{R \cdot Twk}\right)^{-1}\right]^{-1} \cdot \Theta^{(Twk - 293)} \qquad KVHg2 = 0.002849990626771$$

$$KVMhg := \left[KLMhg^{-1} + \left(KGMhg \cdot \frac{HMhg}{R \cdot Twk}\right)^{-1}\right]^{-1} \cdot \Theta^{(Twk - 293)} \qquad KVMhg = 1.979842991876252$$

B-4-12 Diffusion Load to Water Body

$$Ldif := \frac{KVHg2 \cdot 0.48 \cdot Q \cdot Fv \cdot Cywv\_wb \cdot Aw \cdot 1 \cdot 10^{-6}}{\left(\frac{HHg2}{R \cdot Twk}\right)} \qquad Ldif = 0.031498037017449$$

Since this equation describes the dry vapor phase diffusion load to the water body, only the Hg2 value of KV and H are used to calculate Ldif.

$$LdifHg2 := 0.85 \cdot Ldif \qquad LdifHg2 = 0.026773331464832$$

$$LdifMhg := .015 \cdot Ldif \qquad LdifMhg = 0.000472470555262$$

B-4-5 Mercury Loss Constant Due to Leaching

$$ksl := \frac{P + I - RO - Ev}{\Theta sw \cdot Zs \cdot \left[1 + \left(BD \cdot \frac{KdsHg2}{\Theta sw}\right)\right]} \qquad ksl = 0$$

$$ksl := \frac{P + I - RO - Ev}{\Theta sw \cdot Zs \cdot \left[1 + \left(BD \cdot \frac{KdsMhg}{\Theta sw}\right)\right]} \qquad ksl = 0$$

B-4-4 Mercury Loss Constant Due to Runoff

$$ksrHg2 := \frac{RO}{\Theta sw \cdot Zs} \cdot \left[\frac{1}{1 + \left(KdsHg2 \cdot \frac{BD}{\Theta sw}\right)}\right] \qquad ksrHg2 = 0.001149422645005$$

$$ksrMhg := \frac{RO}{\Theta sw \cdot Zs} \cdot \left[\frac{1}{1 + \left(KdsMhg \cdot \frac{BD}{\Theta sw}\right)}\right] \qquad ksrMhg = 0.009523628121369$$

B-4-3 Mercury Loss Constant Due to Soil Erosion

Calculation of this constant has been revised based on EPA Erata dated 08/07/99

$$kseHg2 := \frac{3.1536 \cdot 10^{7} \cdot HHg2}{Zs \cdot KdsHg2 \cdot R \cdot Ta \cdot BD} \qquad kseHg2 = 0.000010525696748$$

$$kseMhg := \frac{3.1536 \cdot 10^{7} \cdot HMhg}{Zs \cdot KdsMhg \cdot R \cdot Ta \cdot BD} \qquad kseMhg = 0.057732493633013$$

B-4-6 Mercury Loss Constant Due to Volatilization

Calculation of this constant has been revised based on EPA Erata dated 08/07/99

$$KeHg2 := \frac{3.1536 \cdot 10^{7} \cdot HHg2}{Zs \cdot KdsHg2 \cdot R \cdot Twk \cdot BD} \qquad KeHg2 = 0.000010525696748$$

$$KeMhg := \frac{3.1536 \cdot 10^{7} \cdot HMhg}{Zs \cdot KdsMhg \cdot R \cdot Twk \cdot BD} \qquad KeMhg = 0.057732493633013$$

$$\Theta vHg2 := 1 - \frac{BD}{Ps} - \Theta sw \qquad \Theta vHg2 = 0.244444444444445$$

$$ktHg2 := \frac{DaHg2 \cdot \Theta vHg2}{Zs} \qquad ktHg2 = 0.011075777777778$$

$$\Theta vMhg := 1 - \frac{BD}{Ps} - \Theta sw \qquad \Theta vMhg = 0.244444444444445$$

$$ktMhg := \frac{DaMhg \cdot \Theta vMhg}{Zs} \qquad ktMhg = 0.012901044444444$$

$$ksvHg2 := KeHg2 \cdot ktHg2 \qquad ksvHg2 = 0.000000116580278$$

$$ksvMhg := KeMhg \cdot ktMhg \qquad ksvMhg = 0.000744809466248$$

B-4-2 Mercury Soil Loss Constant

$$ksHg2 := ksg + kseHg2 + ksrHg2 + ksl + ksvHg2 \qquad ksHg2 = 0.001160064922032$$

$$ksMhg := ksg + kseMhg + ksrMhg + ksl + ksvMhg \qquad ksMhg = 0.06800093122063$$

B-4-1 Wateshed Soil Concentration Due to Deposition

$$Ds := \frac{100\cdot(0.48\cdot Q)}{Zs\cdot BD}\cdot(Fv\cdot(0.31536\cdot Vdv\cdot Cywv + Dywwv) + (Dytwp\_pb\cdot(1 - Fv)))$$ $Ds = 0.000038195493047$

$DsHg2 := Ds\cdot 0.98$ $DsHg2 = 0.000037431583186$

$DsMhg := Ds\cdot 0.02$ $DsMhg = 0.000000763909861$

$$CstDHg2 := \frac{DsHg2\cdot(1 - \exp((-ksHg2\cdot tD)))}{ksHg2}$$ $CstDHg2 = 0.003534200637337$

$$CstDMhg := \frac{DsMhg\cdot(1 - \exp((-ksMhg\cdot tD)))}{ksMhg}$$ $CstDMhg = 0.000011221303924$

B-4-11 Erosion Load to Water Body

$$LeHg2' := Xe\cdot(AL - AI)\cdot SD\cdot ERi\cdot\frac{CstDHg2\cdot KdsHg2\cdot BD}{\Theta sw + KdsHg2\cdot BD}\cdot 0.001$$

$LeHg2' = 24.07338676903389$ $LeHg2 := LeHg2'\cdot 0.85$

$$LeMhg' := Xe\cdot(AL - AI)\cdot SD\cdot ERo\cdot\frac{CstDMhg\cdot KdsMhg\cdot BD}{\Theta sw + KdsMhg\cdot BD}\cdot 0.001$$

$LeMhg' = 0.229299600783856$ $LeMhg := LeMhg' + (LeHg2'\cdot 0.15)$

$LeHg2 = 20.46237875367881$

$LeMhg = 3.840307616138939$

B-4-10 Pervious Runoff load to Water Body

$$LrHg2' := RO\cdot(AL - AI)\cdot\left(\frac{CstDHg2\cdot BD}{\Theta sw + KdsHg2\cdot BD}\right)\cdot 0.01$$

$LrHg2' = 0.34422210510577$ $LrHg2 := 0.85\cdot LrHg2'$ $LrHg2 = 0.292588789339904$

$$LrMhg' := RO\cdot(AL - AI)\cdot\left(\frac{CstDMhg\cdot BD}{\Theta sw + KdsMhg\cdot BD}\right)\cdot 0.01$$

$LrMhg' = 0.009055523465378$ $LrMhg := LrMhg' + (LrHg2'\cdot 0.15)$ $LrMhg = 0.060688839231244$

B-4-9 Impervious Runoff Load to Water Body

$Lri := 0.48\cdot Q\cdot(Fv\cdot Dywwv + (1 - Fv)\cdot Dytwp\_pb)\cdot AI$ $Lri = 0.016214967752824$

$LriHg2 := Lri\cdot 0.85$ $LriHg2 = 0.0137827225899$

$LriMhg := Lri\cdot 0.15$ $LriMhg = 0.002432245162924$

B-4-8 Deposition to Water Body

$$Ldep := 0.48 \cdot Q \cdot (Fv \cdot Dywwv\_wb + (1 - Fv) \cdot Dytwp\_wb\_pb) \cdot Aw$$ $Ldep = 0.029404070364885$

$$LdepHg2 := 0.85 \cdot Ldep$$ $LdepHg2 = 0.024993459810152$

$$LdepMhg := 0.15 \cdot Ldep$$ $LdepMhg = 0.004410610554733$

B-4-7 Total Water Body Load

$$LtHg2 := LdepHg2 + LdifHg2 + LriHg2 + LrHg2 + LeHg2$$ $LtHg2 = 20.8205170568836$

$$LtMhg := LdepMhg + LdifMhg + LriMhg + LrMhg + LeMhg$$ $LtMhg = 3.908311781643101$

B-4-18 Water Column Volatilization Loss Rate Constatn

$$kvHg2 := \frac{KVHg2}{dz \cdot \left(1 + Kdsw \cdot TSS \cdot 10^{-6}\right)}$$ $kvHg2 = 0.00138349059552$

$$kvMhg := \frac{KVMhg}{dz \cdot \left(1 + Kdsw \cdot TSS \cdot 10^{-6}\right)}$$ $kvMhg = 0.961088831007889$

B-4-17 Water Column Volatilization Loss Rate Constatn

$$kwtHg2 := fwcHg2 \cdot kvHg2 + fbsHg2 \cdot kb$$ $kwtHg2 = 0.326372580889599$

$$kwtMhg := fwcMhg \cdot kvMhg + fbsMhg \cdot kb$$ $kwtMhg = 0.340591956693656$

B-4-15 Total Water Body Concentration

$$CwtotHg2 := \frac{LtHg2}{Vfx \cdot fwcHg2 + kwtHg2 \cdot Aw \cdot (dwc + dbs)}$$ $CwtotHg2 = 0.000084689264487$

$$CwtotMhg := \frac{LtMhg}{Vfx \cdot fwcMhg + kwtMhg \cdot Aw \cdot (dwc + dbs)}$$ $CwtotMhg = 0.00001523369761$

B-4-23 Total Water Column Concentration

$$CwctotHg2 := fwcHg2 \cdot CwtotHg2 \cdot \frac{dwc + dbs}{dwc}$$ $CwctotHg2 = 0.000000116150329$

$$CwctotMhg := fwcMhg \cdot CwtotMhg \cdot \frac{dwc + dbs}{dwc}$$ $CwctotMhg = 0.000000341035635$

B-4-24 Dissolved Phase Water Concentration

$$CdwHg2 := \frac{CwctotHg2}{1 + Kdsw \cdot TSS \cdot 10^{-6}}$$ $CdwHg2 = 0.000000058075164$

$$CdwMhg := \frac{CwctotMhg}{1 + Kdsw \cdot TSS \cdot 10^{-6}}$$ $CdwMhg = 0.000000170517818$

B-4-25 Mercury concentration Sorbed to Bed Sediment

$$CsbHg2 := fbsHg2 \cdot CwtotHg2 \cdot \frac{KdbsHg2}{\Theta bs + KdbsHg2 \cdot Cbs} \cdot \frac{dwc + dbs}{dbs}$$ $CsbHg2 = 0.002903758224668$

$$CsbMhg := fbsMhg \cdot CwtotMhg \cdot \frac{KdbsMhg}{\Theta bs + KdbsMhg \cdot Cbs} \cdot \frac{dwc + dbs}{dbs}$$ $CsbMhg = 0.00051155345275$

B-4-27 Fish Concentration from Bioconcentration Factors Using Dissolved Phase Water Concentration

$CfishHg2 := CdwHg2 \cdot BAFfishHg2$ $CfishHg2 = 0$

$CfishMhg := CdwMhg \cdot BAFfishMhg$ $CfishMhg = 1.159521159566327$

$Cfish := CfishHg2 + CfishMhg$ $Cfish = 1.159521159566327$

C-1-4 COPC Intake from Fish

$IfishHg2 := CfishHg2 \cdot CRfish \cdot Ffish$ $IfishHg2 = 0$

$IfishMhg := CfishMhg \cdot CRfish \cdot Ffish$ $IfishMhg = 0.001356639756693$

C-1-5 Mercury Intake from Drinking Water

$$IdwHg2 := \frac{CdwHg2 \cdot CRdwadult \cdot Fdw}{BWadult}$$ $IdwHg2 = 0.000000001161503$

$$IdwMhg := \frac{CdwMhg \cdot CRdwadult \cdot Fdw}{BWadult}$$ $IdwMhg = 0.000000003410356$

C-1-8 Hazard Quotient: Non-carcinogens

$$HQHg2 := \frac{IfishHg2 \cdot ED \cdot EF}{RfD \cdot AT \cdot 365}$$ $HQHg2 = 0$

$$HQMhg := \frac{IfishMhg \cdot ED \cdot EF}{RfD \cdot AT \cdot 365}$$ $HQMhg = 13.00887437924413$