

# Mercury Fate and Transport: Example Calculation

Constants used in this calculation

## Air Model Parameters

Cyvw\_wb := 0.04916806      Cyvw := 0.06139385      Dyvw := 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 :=  $8.205 \cdot 10^{-5}$        $\Theta_{bs}$  := 0.6       $\lambda_z$  := 4      Ta := 298      Yp := 2.24  
 $\mu_w$  :=  $1.69 \cdot 10^{-2}$       P := 100       $\Theta$  := 1.026      a := 1.4       $\mu_a$  :=  $1.81 \cdot 10^{-4}$       Vdv := 3  
 $\rho_w$  := 1      I := 100       $\Theta_{sw}$  := 0.2      b := 0.125       $\rho_a$  :=  $1.2 \cdot 10^{-3}$   
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

$$KG_{Hg2} := (Cd^{0.5} \cdot W) \cdot \frac{k^{0.33}}{\lambda z} \cdot \left( \frac{\mu a}{\rho a \cdot Da_{Hg2}} \right)^{-0.67} \cdot 3.1536 \cdot 10^7 \quad KG_{Hg2} = 86333.54351663143$$

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

### B-4-13 Universal Soil Loss Equation

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

### B-4-14 Sediment Delivery Ratio

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

### B-4-22 Benthic Burial Rate Constant

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

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

$$f_{wcHg2} := \frac{\left( 1 + K_{dsw} \cdot TSS \cdot 10^{-6} \right) \cdot \frac{d_{wc}}{dz}}{\left( 1 + K_{dsw} \cdot TSS \cdot 1 \cdot 10^{-6} \right) \cdot \frac{d_{wc}}{dz} + (\Theta_{bs} + K_{dbsHg2} \cdot Cbs) \cdot \frac{d_{bs}}{dz}} \quad f_{wcHg2} = 0.001331541965542$$

$$f_{wcMhg} := \frac{\left( 1 + K_{dsw} \cdot TSS \cdot 10^{-6} \right) \cdot \frac{d_{wc}}{dz}}{\left( 1 + K_{dsw} \cdot TSS \cdot 1 \cdot 10^{-6} \right) \cdot \frac{d_{wc}}{dz} + (\Theta_{bs} + K_{dbsMhg} \cdot Cbs) \cdot \frac{d_{bs}}{dz}} \quad f_{wcMhg} = 0.02173487795866$$

$$f_{bsHg2} := 1 - f_{wcHg2} \quad f_{bsHg2} = 0.998668458034458 \quad f_{bsMhg} := 1 - f_{wcMhg} \quad f_{bsMhg} = 0.97826512204134$$

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

$$KL_{Hg2} := (Cd^{0.5} \cdot W) \cdot \left( \frac{\rho a}{\rho w} \right)^{0.5} \cdot \frac{k^{0.33}}{\lambda z} \cdot \left( \frac{\mu w}{\rho w \cdot Dw_{Hg2}} \right)^{-0.67} \cdot 3.1536 \cdot 10^7 \quad KL_{Hg2} = 29.87810588409151$$

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

**B-4-19 Overall COPC Transfer Rate Coefficient**

$$KVHg2 := \left[ KLVHg2^{-1} + \left( KGHg2 \cdot \frac{HHg2}{R \cdot Twk} \right)^{-1} \right]^{-1} \cdot \Theta^{(Twk - 293)} \quad KVHg2 = 0.002849990626771$$

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

**B-4-12 Diffusion Load to Water Body**

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

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.

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

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

**B-4-5 Mercury Loss Constant Due to Leaching**

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

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

**B-4-4 Mercury Loss Constant Due to Runoff**

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

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

### 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

$$k_{seHg2} := \frac{3.1536 \cdot 10^7 \cdot HHg2}{Z_s \cdot K_{dsHg2} \cdot R \cdot Ta \cdot BD} \quad k_{seHg2} = 0.000010525696748$$

$$k_{seMhg} := \frac{3.1536 \cdot 10^7 \cdot HMhg}{Z_s \cdot K_{dsMhg} \cdot R \cdot Ta \cdot BD} \quad k_{seMhg} = 0.057732493633013$$

### B-4-6 Mercury Loss Constant Due to Volatilization

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

$$K_{eHg2} := \frac{3.1536 \cdot 10^7 \cdot HHg2}{Z_s \cdot K_{dsHg2} \cdot R \cdot Twk \cdot BD} \quad K_{eHg2} = 0.000010525696748$$

$$K_{eMhg} := \frac{3.1536 \cdot 10^7 \cdot HMhg}{Z_s \cdot K_{dsMhg} \cdot R \cdot Twk \cdot BD} \quad K_{eMhg} = 0.057732493633013$$

$$\Theta_{vHg2} := 1 - \frac{BD}{P_s} - \Theta_{sw} \quad \Theta_{vHg2} = 0.244444444444445$$

$$k_{tHg2} := \frac{D_{aHg2} \cdot \Theta_{vHg2}}{Z_s} \quad k_{tHg2} = 0.011075777777778$$

$$\Theta_{vMhg} := 1 - \frac{BD}{P_s} - \Theta_{sw} \quad \Theta_{vMhg} = 0.244444444444445$$

$$k_{tMhg} := \frac{D_{aMhg} \cdot \Theta_{vMhg}}{Z_s} \quad k_{tMhg} = 0.012901044444444$$

$$k_{svHg2} := K_{eHg2} \cdot k_{tHg2} \quad k_{svHg2} = 0.000000116580278$$

$$k_{svMhg} := K_{eMhg} \cdot k_{tMhg} \quad k_{svMhg} = 0.000744809466248$$

### B-4-2 Mercury Soil Loss Constant

$$k_{sHg2} := k_{sg} + k_{seHg2} + k_{srHg2} + k_{sl} + k_{svHg2} \quad k_{sHg2} = 0.001160064922032$$

$$k_{sMhg} := k_{sg} + k_{seMhg} + k_{srMhg} + k_{sl} + k_{svMhg} \quad k_{sMhg} = 0.06800093122063$$

#### B-4-1 Watershed Soil Concentration Due to Deposition

$$D_s := \frac{100 \cdot (0.48 \cdot Q)}{Z_s \cdot BD} \cdot (F_v \cdot (0.31536 \cdot V_{dv} \cdot C_{ywv} + D_{ywwv}) + (D_{ytwp\_pb} \cdot (1 - F_v))) \quad D_s = 0.000038195493047$$

$$D_{sHg2} := D_s \cdot 0.98 \quad D_{sHg2} = 0.000037431583186$$

$$D_{sMhg} := D_s \cdot 0.02 \quad D_{sMhg} = 0.000000763909861$$

$$C_{stDHg2} := \frac{D_{sHg2} \cdot (1 - \exp((-k_{sHg2} \cdot tD))}{k_{sHg2}} \quad C_{stDHg2} = 0.003534200637337$$

$$C_{stDMhg} := \frac{D_{sMhg} \cdot (1 - \exp((-k_{sMhg} \cdot tD))}{k_{sMhg}} \quad C_{stDMhg} = 0.000011221303924$$

#### B-4-11 Erosion Load to Water Body

$$Le_{Hg2}' := X_e \cdot (AL - AI) \cdot SD \cdot ER_i \cdot \frac{C_{stDHg2} \cdot K_{dsHg2} \cdot BD}{\Theta_{sw} + K_{dsHg2} \cdot BD} \cdot 0.001$$

$$Le_{Hg2}' = 24.07338676903389 \quad Le_{Hg2} := Le_{Hg2}' \cdot 0.85$$

$$Le_{Mhg}' := X_e \cdot (AL - AI) \cdot SD \cdot ER_o \cdot \frac{C_{stDMhg} \cdot K_{dsMhg} \cdot BD}{\Theta_{sw} + K_{dsMhg} \cdot BD} \cdot 0.001$$

$$Le_{Mhg}' = 0.229299600783856 \quad Le_{Mhg} := Le_{Mhg}' + (Le_{Hg2}' \cdot 0.15)$$

$$Le_{Hg2} = 20.46237875367881$$

$$Le_{Mhg} = 3.840307616138939$$

#### B-4-10 Pervious Runoff load to Water Body

$$Lr_{Hg2}' := RO \cdot (AL - AI) \cdot \left\{ \frac{C_{stDHg2} \cdot BD}{\Theta_{sw} + K_{dsHg2} \cdot BD} \right\} \cdot 0.01$$

$$Lr_{Hg2}' = 0.34422210510577 \quad Lr_{Hg2} := 0.85 \cdot Lr_{Hg2}' \quad Lr_{Hg2} = 0.292588789339904$$

$$Lr_{Mhg}' := RO \cdot (AL - AI) \cdot \left\{ \frac{C_{stDMhg} \cdot BD}{\Theta_{sw} + K_{dsMhg} \cdot BD} \right\} \cdot 0.01$$

$$Lr_{Mhg}' = 0.009055523465378 \quad Lr_{Mhg} := Lr_{Mhg}' + (Lr_{Hg2}' \cdot 0.15) \quad Lr_{Mhg} = 0.060688839231244$$

#### B-4-9 Impervious Runoff Load to Water Body

$$Lr_i := 0.48 \cdot Q \cdot (F_v \cdot D_{ywwv} + (1 - F_v) \cdot D_{ytwp\_pb}) \cdot AI \quad Lr_i = 0.016214967752824$$

$$Lr_{iHg2} := Lr_i \cdot 0.85 \quad Lr_{iHg2} = 0.0137827225899$$

$$Lr_{iMhg} := Lr_i \cdot 0.15 \quad Lr_{iMhg} = 0.002432245162924$$

#### B-4-8 Deposition to Water Body

$$L_{dep} := 0.48 \cdot Q \cdot (F_v \cdot Dy_{wvw\_wb} + (1 - F_v) \cdot Dy_{twp\_wb\_pb}) \cdot A_w \quad L_{dep} = 0.029404070364885$$

$$L_{depHg2} := 0.85 \cdot L_{dep} \quad L_{depHg2} = 0.024993459810152$$

$$L_{depMhg} := 0.15 \cdot L_{dep} \quad L_{depMhg} = 0.004410610554733$$

#### B-4-7 Total Water Body Load

$$L_{tHg2} := L_{depHg2} + L_{difHg2} + L_{riHg2} + L_{rHg2} + L_{eHg2} \quad L_{tHg2} = 20.8205170568836$$

$$L_{tMhg} := L_{depMhg} + L_{difMhg} + L_{riMhg} + L_{rMhg} + L_{eMhg} \quad L_{tMhg} = 3.908311781643101$$

#### B-4-18 Water Column Volatilization Loss Rate Constant

$$k_{vHg2} := \frac{K_{VHg2}}{dz \cdot (1 + K_{dsw} \cdot TSS \cdot 10^{-6})} \quad k_{vHg2} = 0.00138349059552$$

$$k_{vMhg} := \frac{K_{VMhg}}{dz \cdot (1 + K_{dsw} \cdot TSS \cdot 10^{-6})} \quad k_{vMhg} = 0.961088831007889$$

#### B-4-17 Water Column Volatilization Loss Rate Constant

$$k_{wtHg2} := f_{wcHg2} \cdot k_{vHg2} + f_{bsHg2} \cdot k_b \quad k_{wtHg2} = 0.326372580889599$$

$$k_{wtMhg} := f_{wcMhg} \cdot k_{vMhg} + f_{bsMhg} \cdot k_b \quad k_{wtMhg} = 0.340591956693656$$

#### B-4-15 Total Water Body Concentration

$$C_{wtotHg2} := \frac{L_{tHg2}}{V_f \cdot f_{wcHg2} + k_{wtHg2} \cdot A_w \cdot (dwc + dbs)} \quad C_{wtotHg2} = 0.000084689264487$$

$$C_{wtotMhg} := \frac{L_{tMhg}}{V_f \cdot f_{wcMhg} + k_{wtMhg} \cdot A_w \cdot (dwc + dbs)} \quad C_{wtotMhg} = 0.00001523369761$$

#### B-4-23 Total Water Column Concentration

$$C_{wctotHg2} := f_{wcHg2} \cdot C_{wtotHg2} \cdot \frac{dwc + dbs}{dwc} \quad C_{wctotHg2} = 0.000000116150329$$

$$C_{wctotMhg} := f_{wcMhg} \cdot C_{wtotMhg} \cdot \frac{dwc + dbs}{dwc} \quad C_{wctotMhg} = 0.000000341035635$$

**B-4-24 Dissolved Phase Water Concentration**

$$C_{dwHg2} := \frac{C_{wtotHg2}}{1 + K_{dsw} \cdot TSS \cdot 10^{-6}} \quad C_{dwHg2} = 0.000000058075164$$

$$C_{dwMhg} := \frac{C_{wtotMhg}}{1 + K_{dsw} \cdot TSS \cdot 10^{-6}} \quad C_{dwMhg} = 0.000000170517818$$

**B-4-25 Mercury concentration Sorbed to Bed Sediment**

$$C_{sbHg2} := f_{bsHg2} \cdot C_{wtotHg2} \cdot \frac{K_{dbsHg2}}{\Theta_{bs} + K_{dbsHg2} \cdot C_{bs}} \cdot \frac{d_{wc} + d_{bs}}{d_{bs}} \quad C_{sbHg2} = 0.002903758224668$$

$$C_{sbMhg} := f_{bsMhg} \cdot C_{wtotMhg} \cdot \frac{K_{dbsMhg}}{\Theta_{bs} + K_{dbsMhg} \cdot C_{bs}} \cdot \frac{d_{wc} + d_{bs}}{d_{bs}} \quad C_{sbMhg} = 0.00051155345275$$

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

$$C_{fishHg2} := C_{dwHg2} \cdot BAF_{fishHg2} \quad C_{fishHg2} = 0$$

$$C_{fishMhg} := C_{dwMhg} \cdot BAF_{fishMhg} \quad C_{fishMhg} = 1.159521159566327$$

$$C_{fish} := C_{fishHg2} + C_{fishMhg} \quad C_{fish} = 1.159521159566327$$

**C-1-4 COPC Intake from Fish**

$$I_{fishHg2} := C_{fishHg2} \cdot CR_{fish} \cdot F_{fish} \quad I_{fishHg2} = 0$$

$$I_{fishMhg} := C_{fishMhg} \cdot CR_{fish} \cdot F_{fish} \quad I_{fishMhg} = 0.001356639756693$$

**C-1-5 Mercury Intake from Drinking Water**

$$I_{dwHg2} := \frac{C_{dwHg2} \cdot CR_{dwadult} \cdot F_{dw}}{BW_{adult}} \quad I_{dwHg2} = 0.000000001161503$$

$$I_{dwMhg} := \frac{C_{dwMhg} \cdot CR_{dwadult} \cdot F_{dw}}{BW_{adult}} \quad I_{dwMhg} = 0.000000003410356$$

**C-1-8 Hazard Quotient: Non-carcinogens**

$$HQ_{Hg2} := \frac{I_{fishHg2} \cdot ED \cdot EF}{RfD \cdot AT \cdot 365} \quad HQ_{Hg2} = 0$$

$$HQ_{Mhg} := \frac{I_{fishMhg} \cdot ED \cdot EF}{RfD \cdot AT \cdot 365} \quad HQ_{Mhg} = 13.00887437924413$$