MEMORANDUM

Date: July 20, 1999

To: David Layland EPA/OSW/EMRAD

From: Miriam Gilkinson

Subject: Sample Calculation for Mercury in Support of the HWC Background Document

The following provides a sample calculation of indirect exposures following the outline provided in *Human Health and Ecological Risk Assessment Support to the Development of Technical Standards for Emissions from Combustion Units Burning Hazardous Wastes: Background Document, Final Report, July 1999, Appendix C*. Sources of equations and variable values are documented in Appendix D of the same report.

The sample calculation is provided for Site 321, Sector 7, Waterbody 3 (Lake Demopolis) for the adult (>19-yr-old) subsistence fisher scenario. The calculation follows all mercury species, including modified transformation in soils.

The equations that follow were used to calculate sector soil concentrations used to evaluate mercury exposure through soil ingestion. Lyon et al. used the atmospheric deposition values to perform the waterbody modeling and provided waterbody media concentrations and a fish tissue concentration, used to estimate mercury exposure through fish ingestion (Lyon, B., M.R. Gilkinson, and T.B. Marimpietri. 1998. *Application of the IEM-2M Surface Water Model to Airborne Mercury Deposited From Hazardous Waste Combustors*. Lyon Technical Consulting, Knoxville, TN). Because the receptor used in this sample calculation is the subsistence fisher, the equations for terrestrial food chain concentrations are not shown: this receptor is modeled to be exposed through inhalation and sector soil, fish, and drinking water ingestion. Furthermore, because Lake Demopolis is not used for drinking water, the drinking water calculations do not apply for this sample calculation.

The endpoint of these calculations (shown in Tables 13 and 14) is hazard quotients for indirect and direct exposure to mercury. The equations used to calculate the hazard quotients are presented in Tables 2 through 12. Equations are presented so that the media concentration (i.e., soil concentration) is first, followed by all required supporting subcalculations. To allow the reader to duplicate the original spreadsheet calculations, many of the following numerical values have been shown to multiple decimal places. If these numbers are rounded, the calculations will no longer yield the same results as the spreadsheet model. The results of this sample calculation can be compared to the pathway-specific risk results found in Section IX of the Risk Results. Specifically, the results are found in Table IX-B14, *Individual Risks and Hazard Quotients by*

Pathway for the Subsistence Fisher, Baseline: Cement Kiln (Stack Number 321) - Sector 7. Note that the results presented in this table contain only one significant digit.

The following table contains the outputs from the ISCST3 model. These outputs were combined as indicated to form to values used as inputs in IEM-2M. The input values can be found in Table G-3, *Site-Specific Inputs Used for Baseline* of the report *Human Health and Ecological Risk Assessment Support to the Development of Technical Standards for Emissions from Combustion Units Burning Hazardous Wastes: Background Document, Final Report, July 1999, Appendix G*.

Table 1. ISCST3 Outputs/IEM-2M Inputs

Parameter	Value	Units
Divalent mercury watershed air concentration	0.0000267709391488434	μg/m^3
Elemental mercury watershed air concentration	4.37621765601218E-06	μg/m^3
Total mercury watershed air concentration	**0.0000311471568048556**	**μg/m^3**
Divalent mercury combined watershed particle deposition rate	1.37098491048999E-08	g/m^2-yr
Divalent mercury watershed wet vapor deposition rate	4.40793827114822E-06	g/m^2-yr
Divalent mercury watershed dry vapor deposition rate	0.0000140286435535872	g/m^2-yr
Divalent mercury watershed deposition load	**0.0000184502916738403**	**g/m^2-yr**
Elemental mercury watershed combined particle deposition rate	0	g/m^2-yr
Elemental mercury watershed wet vapor deposition rate	6.21765601217656E-08	g/m^2-yr
Elemental mercury watershed deposition load	**6.21765601217656E-08**	**g/m^2-yr**
Combined divalent mercury waterbody particle deposition rate	7.67600892191921E-08	g/m^2-yr
Divalent mercury waterbody wet vapor deposition rate	0.0000591018913442487	g/m^2-yr
Divalent mercury waterbody deposition load	**0.0000591786514334679**	**g/m^2-yr**
Combined elemental mercury waterbody particle deposition rate	0	g/m^2-yr
Elemental mercury waterbody wet vapor deposition rate	2.81963470319635E-07	g/m^2-yr
Elemental mercury waterbody deposition load	**2.81963470319635E-07**	**g/m^2-yr**
Divalent mercury waterbody air concentration	0.0000409145923205235	μg/m^3
Elemental mercury waterbody air concentration	6.61168188736682E-06	μg/m^3
Total mercury waterbody air concentration	**0.0000475262742078903**	**μg/m^3**

The equation in Table 2 calculates a soil concentration for total mercury and the three mercury species at time T as a result of wet and dry deposition of particles and vapors to soil. Only divalent and elemental mercury are assumed to be deposited onto the soil. The background soil concentration and internal transformation load are assumed to be zero for all species. Vapor and particulate deposition rates were output from ISCST3.

Table 2. Mercury Soil Concentration Due to Deposition

$$Sc = \frac{L_w}{ks \bullet Z \bullet BD} (1 - e^{-ks \bullet Tc})\, 100 + C_{sb}$$

$$L_w = \sum_i L_{w,i}$$

$$L_{w,i} = D_{TDW,i} + D_{WVW,i} + L_{IS,i} + L_{Dif,i}$$

$$Sc_i = Sc \bullet fs_i$$

Parameter Name and Definition		Species	Value(s)
Sc	Average soil concentration of total mercury in soil (µg/g)		0.426386397003035
L_w	Load of total mercury to soil on an areal basis (g/m^2-yr)		0.000279320172503011
ks	Soil loss constant for total mercury (yr^{-1}) [see Table 5]		0.0189014404402988
Z	Mixing depth of soil (cm)		1
BD	Bulk density of soil (g/cm^3)		1.5
Tc	Time period of combustion		30
C_{sb}	Background "natural" soil concentration (µg/g)		0
$L_{w,i}$	Load of the ith species to soil on an areal basis (g/m^2-yr)	Divalent Elemental	0.000278524890920058 7.95281582952816E-07
$D_{TDW,i}$	Total (wet and dry) deposition of particles to the soil (g/m^2-yr)	Divalent Elemental	2.51359788396704E-07 0
$D_{WVW,i}$	Wet deposition of mercury vapors to soil (g/m^2-yr)	Divalent Elemental	0.00026065122586831 7.95281582952816E-07
$L_{IS,i}$	Internal transformation load (g/m^2-yr)		0
$L_{Dif,i}$	Diffusion flux of mercury to soil (g/m^2-yr) [see Table 4]	Divalent Elemental	0.0000176223052633511 0
Sc_i	Soil concentration of the ith mercury species (µg/g)	Divalent Elemental Methyl	0.4178558299042 2.83915877426754E-06 0.00852772794006069
fs_i	Equilibrium fraction of the ith mercury species in soil [see Table 3]	Divalent Elemental Methyl	0.979993341347674 6.65865232620761E-06 0.02

The equations in Table 3 calculates an equilibrium soil fraction for each of the three mercury species. Methylmercury is assumed to be constant at 2 percent, and elemental and divalent mercury are assumed to make up the other 98 percent. The relative concentrations of elemental and divalent mercury are assumed to be related through the relative transformation rates for each species (volatilization and reduction, respectively).

Table 3. Equilibrium Fraction of the i^{th} Species in Soil

$$fs_{elemental} = \frac{ks_{red} \bullet 365}{ksv_{elemental}} \bullet fs_{divalent}$$

$$fs_{methyl} = 0.02 \qquad fs_{divalent} + fs_{elemental} = 0.98$$

Parameter Name and Definition		Species	Value(s)
$fs_{divalent}$ $fs_{elemental}$ fs_{methyl}	Equilibrium fraction of the i^{th} mercury species in soil	Divalent Elemental Methyl	0.979993341347674 6.65865232620761E-06 0.02
ks_{red}	Divalent mercury reduction rate constant (d^{-1})		0.00005
365	Units conversion factor (d/yr)		
$ksv_{elemental}$	Soil loss constant due to volatilization for elemental mercury (yr^{-1}) [see Table 8]		2685.96070246864

The equation in Table 4 calculates the diffusion flux of divalent and elemental mercury to soil. Because no methylmercury was assumed to be emitted from hazardous waste combustors, no flux occurs for methylmercury. Per the 1997 *Mercury Study Report to Congress, Volume III - Fate and Transport of Mercury in the Environment* (U.S. EPA, Office of Air Quality Planning and Standards and Office of Research and Development, Washington, DC, EPA 452/R-97/005), the dry deposition velocity of elemental mercury is though to be negligible. Therefore, divalent mercury is the only species with a site-specific dry deposition velocity and, therefore, it is the only species that contributes a diffusion flux to the soil.

Table 4. Atmospheric Diffusion Flux to Soil

$$L_{Dif,i} = 0.31536 \bullet K_{t,i} \bullet C_{vws,i}$$

Parameter Name and Definition		Species	Value(s)
$L_{Dif,i}$	Diffusion flux of the i^{th} species to soil (g/m^2-yr)	Divalent Elemental	0.0000176223052633511 0
0.31536	Units conversion factor (m-g-s/cm-µg-yr)		
$K_{t,i}$	Dry deposition velocity for the i^{th} species (cm/s)	Divalent Elemental	1.66167263100237 0
$C_{vws,i}$	Average vapor phase air concentration ($\mu g/m^3$)	Divalent Elemental	0.0000336287439384603 0.0000053826103500761

The equation in Table 5 calculates the soil loss constant, which accounts for the loss of contaminant from soil by several mechanisms. These mechanisms include leaching, surface runoff, degradation, and volatilization. Erosion and degradation losses are assumed to be zero.

Table 5. Soil Loss Constant

$$ks = \sum ks_i \cdot fs_i$$

$$ks_i = ksl_i + ksr_i + ksv_i + kse_i + ksg_i$$

Parameter Name and Definition		Species	Sector Value(s)
ks	Soil loss constant for total mercury (yr^{-1})		0.0189014404402988
ks_i	Soil loss constant due to all processes for the i^{th} mercury species (yr^{-1})	Divalent Elemental Methyl	0.000458422944536009 2685.98701868252 0.0283567648509334
fs_i	Equilibrium fraction of the i^{th} mercury species in soils [see Table 3]	Divalent Elemental Methyl	0.979993341347674 6.65865232620761E-06 0.02
ksl_i	Loss constant due to leaching for the i^{th} mercury species (yr^{-1}) [see Table 6]	Divalent Elemental Methyl	0.000161838679015482 0.00938531639899338 0.00134092482107113
ksr_i	Loss constant due to surface runoff for the i^{th} mercury species (yr^{-1}) [see Table 7]	Divalent Elemental Methyl	0.000291953298792133 0.0169308974811386 0.0024189979016482
ksv_i	Loss constant due to volatilization for the i^{th} species (yr^{-1}) [see Table 8]	Divalent Elemental Methyl	4.63096672839421E-06 2685.96070246864 0.0245968421282141
kse_i	Loss constant due to soil erosion (yr^{-1})		0
ksg_i	Loss constant due to degradation (yr^{-1})		0

Table 6 contains the specific equation used to calculate the species-specific loss constant due to leaching from soil.

Table 6. Loss Constant Due to Leaching

$$ksl_i = \frac{P + I - R - E_v}{\theta_s \bullet Z \bullet [1.0 + (BD \bullet Kd_{s,i}/\theta_s)]}$$

Parameter Name and Definition		Species	Value(s)
ksl_i	Loss constant due to leaching for the i^{th} mercury species (yr^{-1})	Divalent Elemental Methyl	0.000161838679015482 0.00938531639899338 0.00134092482107113
P	Average annual precipitation (cm/yr)		131.6
I	Average annual irrigation (cm/yr)		0
R	Average annual runoff (cm/yr)		25.4
E_v	Average annual evapotranspiration (cm/yr)		92.12
θ_s	Soil volumetric water content (mL/cm^3)		0.215805352087004
Z	Soil depth (cm)		1
BD	Soil bulk density (g/cm^3)		1.5
$Kd_{s,i}$	Soil-water partition coefficient for the i^{th} mercury species (cm^3/g)	Divalent Elemental Methyl	58,000 1,000 7,000

The equation in Table 7 calculates the contaminant loss constant due to runoff from soil.

Table 7. Loss Constant Due to Runoff

$$ksr_i = \frac{R}{\theta_s \bullet Z}\left(\frac{1}{1 + (Kd_{s,i} \bullet BD/\theta_s)}\right)$$

Parameter Name and Definition		Species	Sector Value(s)
ksr_i	Loss constant due to runoff for the i^{th} species (yr^{-1})	Divalent Elemental Methyl	0.000291953298792133 0.0169308974811386 0.0024189979016482
R	Average annual runoff (cm/yr)		25.4
θ_s	Soil volumetric water content (mL/cm^3)		0.215805352087004
Z	Soil mixing depth (cm)		1
$Kd_{s,i}$	Soil-water partition coefficient for the i^{th} species (cm^3/g)	Divalent Elemental Methyl	58,000 1,000 7,000
BD	Soil bulk density (g/cm^3)		1.5

Table 8 presents an equation to calculate the contaminant loss constant due to volatilization from soil.

Table 8. Loss Constant Due to Volatilization

$$ksv_i = \left[\frac{3.1536 \times 10^7 \bullet H_i}{Z \bullet Kd_{s,i} \bullet R \bullet T \bullet BD}\right] \bullet \left[0.482 \bullet u^{0.78} \bullet \left(\frac{\mu_a}{\rho_a \bullet Da_i}\right)^{-0.67} \bullet \left(\sqrt{\frac{4 \bullet A}{\pi}}\right)^{-0.11}\right]$$

	Parameter Name and Definition	Species	Value(s)
ksv_i	Loss constant due to volatilization for i^{th} mercury species (yr^{-1})	Divalent Elemental Methyl	4.63096672839421E-06 2685.96070246864 0.0245968421282141
3.1536×10^7	Units conversion factor (s/yr)		
H_i	Henry's law constant (atm-m^3/mol)	Divalent Elemental Methyl	0.00000000071 0.0071 0.00000047
Z	Soil mixing depth (cm)		1
$Kd_{s,i}$	Soil-water partition coefficient (cm^3/g)	Divalent Elemental Methyl	58,000 1,000 7,000
R	Universal gas constant (atm-m^3/mol-K)		0.00008205
T	Ambient air temperature (K)		291.483333333333
BD	Soil bulk density (g/cm^3)		1.5
u	Average annual wind speed (m/s)		3.584
μ_a	Viscosity of air (g/cm-s)		0.000181
ρ_a	Density of air (g/cm^3)		0.00119
Da_i	Diffusivity of the i^{th} mercury species in air (cm^2/s)	Divalent Elemental Methyl	0.0553719174379913 0.0553719174379913 0.0527777777777778
A	Surface area of contaminated area (m^2)		2,024

Air concentration for direct inhalation was calculated from the sum of both the vapor phase and particle phase concentrations, as seen in Table 9. Risks of direct inhalation were calculated for species emitted by the combustion source that had inhalation health criteria or benchmarks. Although both divalent and elemental mercury are both emitted (as shown in Table 12), only elemental mercury has a reference concentration (RfC). Therefore, inhalation risks ultimately are determined for elemental mercury only.

Table 9. Air Concentration for Inhalation

$$Ca = Q \bullet [\,(Fv \bullet Cyv) + (1.0 - Fv) \bullet Cyp\,]$$

Parameter Name and Definition		Species	Value(s)
Ca	Total air concentration (µg/m^3)	Divalent Elemental	0.0000337203689190167 0.0000053826103500761
Q	Stack emissions (g/s)	Divalent Elemental	0.0045662100456621 0.000722983257229833
Fv	Fraction of air concentration in vapor phase (dimensionless)	Divalent Elemental	0.997250497294896 1
Cyv	Normalized vapor phase air concentration (µg-s/g-m^3)	Divalent Elemental	0.007385 0.007445
Cyp	Normalized particle phase air concentration (µg-s/g-m^3)	Divalent Elemental	0.007298 0.007298

The equation shown in Table 10 calculates the daily intake of mercury from soil consumption. A small quantity of soil is assumed to be incidentally ingested daily.

Table 10. Contaminant Intake from Soil

$$I_{soil,i} = Sc_i \bullet CR_{soil} \bullet F_{soil}$$

Parameter Name and Definition		Species	Value(s)
Aecial	Daily intake of the i^{th} mercury species from soil (mg/d)	Divalent Elemental Methyl	0.00002089279149521 1.41957938713377E-10 4.26386397003035E-07
Sci.	Sector soil concentration of the i^{th} mercury species (µg/g) [see Table 2]	Divalent Elemental Methyl	0.4178558299042 2.83915877426754E-06 0.00852772794006069
CR_{soil}	Consumption rate of soil (kg/d)		0.00005
F_{soil}	Fraction of consumed soil contaminated (unitless)		1

Table 11 presents the equation to calculate the daily intake of methylmercury from ingestion of fish. The methylmercury concentration in fish varies for each waterbody. Fish tissue concentrations were calculated by Lyon et al. (1998) based on ISCST3 output (see Table 1).

Table 11. Methylmercury Intake from Fish

$$I_{fish} = C_{fish} \bullet CR_{fish} \bullet F_{fish}$$

Parameter Name and Definition		Value(s)
I_{fish}	Daily intake of methylmercury from fish (mg/d)	0.00746446162729134
C_{fish}	Concentration of methylmercury in fish (mg/kg)	0.106635166104162
CR_{fish}	Consumption rate of fish (kg/d)	0.07
F_{fish}	Fraction of fish contaminated (unitless)	1

The equation in Table 12 calculates the daily intake of each mercury species via all indirect pathways. For the sample calculation presented herein, the chosen receptor (the subsistence fisher) is exposed through only two indirect pathways: soil ingestion and fish ingestion. The hazard quotients for indirect exposure and direct exposure are calculated as shown in Tables 13 and 14, respectively.

Table 12. Total Daily Indirect Intake of Mercury Species

$$I_i = I_{soil,i} + I_{fish,i}$$

Parameter Name and Definition		Species	Value(s)
I_i	Total daily intake of the i^{th} mercury species (mg/d)	Divalent Elemental Methyl	0.00002089279149521 1.41957938713377E-10 0.00746488801368834
$I_{soil,\,i}$	Daily intake of the i^{th} mercury species from soil (mg/d)	Divalent Elemental Methyl	0.00002089279149521 1.41957938713377E-10 4.26386397003035E-07
I_{fish}	Daily intake methylmercury from fish (mg/d)	Methyl	0.00746446162729134

The equation in Table 13 calculates the average daily dose (ADD) and hazard quotient (HQ) for indirect exposure to mercury. These are not calculated for elemental mercury because it does not have a reference dose (RfD). Note that these values correspond to those in Section IX of the Risk Results.

Table 13. Hazard Quotient from Indirect Exposure

$$ADD_i = \frac{I_i}{BW} \qquad HQ_i = \frac{ADD_i}{RfD_i}$$

Parameter Name and Definition		Species	Value(s)
ADD_i	Average daily dose of the i^{th} mercury species (mg/kg/d)	Divalent Elemental Methyl	2.90985953972284E-07 1.97713006564592E-12 0.000103967799633542
I_i	Total daily intake of the i^{th} mercury species (mg/d)	Divalent Elemental Methyl	0.00002089279149521 1.41957938713377E-10 0.00746488801368834
BW	Body weight (kg)		71.8
HQ_i	Hazard quotient of the i^{th} mercury species (unitless)	Divalent Methyl (d) Methyl (n)	0.000969953179907613 1.03967799633542 0.346559332111807
RfD_i	Reference dose for divalent mercury (mg/kg/d)		0.0003
RfD_i	Reference dose for developmental effects (d) from exposure to methylmercury (mg/kg/d)		0.0001
RfD_i	Reference dose for neurological effects (n) from exposure to methylmercury (mg/kg/d)		0.0003

Table 14 presents the equation to calculate the hazard quotient for direct inhalation of elemental mercury, the only species for which a reference concentration (RfC) was available.

Table 14. Hazard Quotient Due to Direct Inhalation of Elemental Mercury

$$HQ = \frac{Ca}{RfC} \bullet 10^{-3}$$

Parameter Name and Definition		Value(s)
HQ	Hazard quotient via inhalation of elemental mercury	0.0000179420345002537
Ca	Total air concentration of elemental mercury (µg/m³) [see Table 9]	0.0000053826103500761
RfC	Reference concentration (mg/m³)	0.0003
10^{-3}	Units conversion factor (mg/m³)	