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Polychlorinated Biphenyl Congeners: Analytical Co-elution and the Development of Toxic Equivalency Factors (TEQ) for Housatonic River Biota Tissue Samples

SITE: GE-Housatonic
BREAK: 2.2
OTHER: 212365

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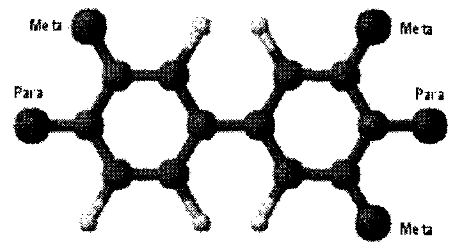
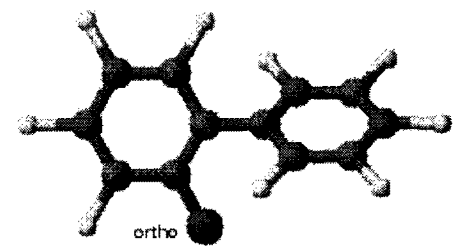
OVERVIEW & PURPOSE

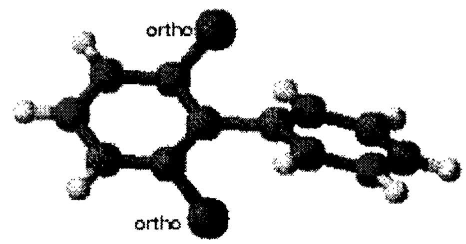
To estimate toxic equivalents (TEQs) in the diet of predators in the Housatonic primary study area, congener-specific concentrations data are required for the primary co-planar PCBs, dioxins and furans in prey tissues. In tissue samples analyzed by the Geochemical and Environmental Research Group (GERG), however, several of the congeners required for TEQ calculations were co-eluted with other congeners. Specifically, PCB-123 co-eluted with PCB-149 to form the doublet PCB-123/149. PCB-157 co-eluted with PCB-201 and PCB-173 to form the triplet PCB-201/157/173. The co-elution of these congeners was a result of the use of a single analytical column that was unable to resolve all of the individual congeners. When developing TEQs, assuming that the concentration of the congener PCB-123 is equal to the doublet concentration and that the concentration of PCB-157 is equal to the triplet concentration would lead to a overestimate of the TEQ value. Conversely, assuming that concentrations of the two congeners (*i.e.*, PCB-123 and PCB-157) were equal to zero would lead to an underestimate of the TEQ value. These two approaches are useful to estimate TEQ bounds, but say little about the relative probabilities of values between the bounds. The purpose of this paper is to develop an approach for estimating concentrations of congeners PCB-123 and PCB-157 in prey tissues that were analyzed by GERG.



para-meta coplanar PCB



mono-ortho coplanar PCB



di-ortho coplanar PCB

Figure 1. Structural diagrams of examples of different coplanar PCBs

Polychlorinated Biphenyls

Polychlorinated Biphenyls (PCBs) are anthropogenic synthetic organic chemicals. They are created when chlorine atoms replace hydrogen atoms on a biphenyl structure. The biphenyl structure is composed of two benzene rings, joined by a single carbon-carbon bond. There are ten positions where chlorine atoms can join on the biphenyl structure. As a result, there are 209 variations, or congeners, that can be created.

Congeners

Only about 130 of the 209 congeners occur in synthesized mixtures of PCBs (USEPA 2001; McFarland and Clarke 1989). Congeners are named according to the total number and location of chlorine atoms on the biphenyl rings. The different arrangements of congeners are categorized into subgroups called homologs. Each homolog contains congeners with the same relative number of chlorine atoms (USEPA 2001). The number of chlorine atoms a congener contains influences how it reacts in the environment and its relative toxicity. For example, congeners with five to seven chlorine atoms appear to be accumulated to the greatest extent. Less chlorinated congeners are metabolized more quickly and highly chlorinated congeners are too large to diffuse through biological membranes (Environment Canada 1997).

Congeners can be grouped based on toxicity and ability to induce mixed-function oxidase systems (MFOs). Coplanar congeners (Figure 1) appear to be the most toxicologically active congeners in commercial PCB mixtures. Congeners from this group have chlorine substitutions at both para- positions and at least two of the meta- positions, with none on the ortho- positions. The second structural group is the mono-ortho coplanar congeners. This group is characterized by having a single ortho-chlorine substitution. Di-ortho coplanar congeners represent a third structural group. These congeners tend to exhibit fewer toxicological effects (McFarland *et al.* 1989; Safe 1994).

Aroclors

In the environment, PCBs are usually found as mixtures of congeners. Mixtures made by the Monsanto Company are known by the trade name Aroclor. Other commercial trade names of PCB mixtures manufactured outside of the United States include Kanechlor, Clophen, Fenclor, and Phenclor (ATSDR 1997). The congener make-up of each Aroclor determines the physical-chemical properties of the mixture. Aroclors are defined by a four digit number. The first two digits are usually 12. The last two digits represent the percentage by weight of chlorine in the mixture (Environment Canada 1997). For example, Aroclor 1254 contains 54% chlorine by weight. Aroclor 1016 is an exception to this rule. Aroclor 1016 is an exception to this rule. It is a re-distilled version of Aroclor 1242 and contains 41% chlorine (Safe 1994). Appendix 1 lists the congeners that are present in the two Aroclors (1260 and 1254a) that were used at the Pittsfield GE facility.

TOXIC EQUIVALENCY FACTORS (TEFS) AND TOXIC EQUIVALENTS (TEQ)

PCBs belong to a large class of chemicals called planar chlorinated hydrocarbons (PCH) that are regularly detected in the environment. The PCHs also include polychlorinated dibenzo-*p*-dioxins (PCDD), and polychlorinated dibenzo-*p*-furans (PCDF). PCHs have a common structural relationship that includes

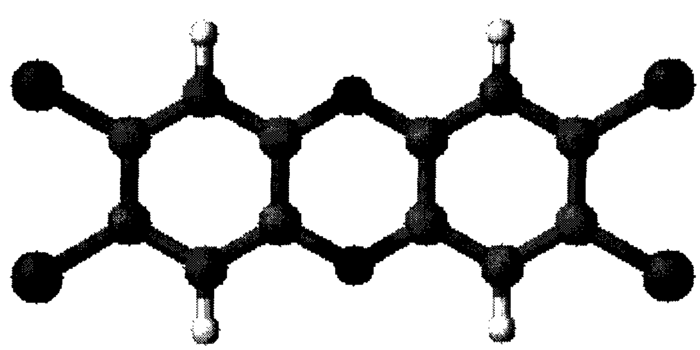


Figure 2. Molecular structure of the planar chlorinated hydrocarbon, 2,3,7,8-tetrachlorodibenzo-p-dioxin

lateral halogenation (*i.e.*, the addition of a halogen such as fluorine or chlorine to a compound), and the ability to assume a planar conformation (Figure 2). This structure is important as it leads to a common mechanism of action in many animal species that involves binding to the aryl hydrocarbon (Ah) receptor and elicitation of an Ah receptor-mediated biochemical and toxic response (Van den Berg *et al.* 1998; Newsted *et al.* 1995; Safe 1994). These responses may lead to lethality, hepatic lesions, immunotoxicity, tumor promotion, adverse effects on reproduction, and induction of drug-metabolizing enzymes (Van den Berg *et al.* 1998; Newsted *et al.* 1995). The planar conformation is the key to the ability of the the chemical to bind with the aryl hydrocarbon (Ah) receptor (Birnbaum & Devito 1995; Newsted *et al.* 1995). This Ah-receptor facilitates the translocation of PCHs into the nucleus of affected cells and the binding of the PCH-Ah receptor complex to sites on the DNA (Newsted *et al.* 1995).

Environmental degradation of PCH congeners varies due to their unique physical/chemical properties (Colgiano 1998). These can cause substantial differences between the congeners detected in environmental samples and the congener makeup of the original product or Aroclor (Coligiano 1998; Van den Berg *et al.* 1998). Additionally, each of the congeners themselves has different potencies, there may be synergistic and/or antagonisitic effects amongst the congeners, and there are differences in the sensitivities of exposed species to the PCH mixtures. To address these issues and effectively estimate the relative toxicity of these mixtures, a system has been created involving the development and use of toxic equivalency factors (TEFs). This approach is based on the *in vivo* and *in vitro* toxicity of each of the PCH congeners in relation to 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD). TCDD is considered to be the most toxic member of the PCH class of chemicals (Van den Berg *et al.* 1998; Birnbaum & DeVito 1995; Safe 1994). There are a number of assumptions made when using the TEF approach. These include: 1. PCH congeners are Ah-receptor antagonists and their toxicological potency is mediated by their binding affinity; 2. no interaction occurs between the congeners and thus the sum of the individual congener effects accounts for the potency of the PCH mixture. The overall effect of these assumptions is a potency estimate or toxic equivalent (TEQ) value. To generate a TEQ the following equation (Equation 1- modified from Van den Berg *et al.* 1998) is used:

$$TEQ = \sum_{n=1}^{6}[PCDD_n \ x \ TEF_n] + \sum_{p=1}^{10}[PCDF_p \ x \ TEF_p] + \sum_{q=1}^{12}[PCB_q \ x \ TEF_q] \quad \textbf{EQ. 1}$$

where,

TEQ – Toxic equivalent
$PCDD_n$ – Polychloronated dibenzo-p-dioxin congener concentration
$PCDF_p$ – Polychloronated dibenzo-p-furan congener concentration
PCB_q – Polychlorinated biphenyl congener concentration
$TEF_{n,p,q}$ – Toxic equivalency factor for appropriate individual PCDD/PCDF and PCB congeners, respectively.

There are a number of TEF schemes available in the scientific literature for PCHs (Van den Berg *et al.* 1998; Kennedy *et al.* 1996 ; Safe 1994). For the purposes of this report the TEFs presented by Van den Berg *et al.* (1998) have been adopted. TEF values are developed for those compounds that: 1. show a structural relationship to PCDDs and PCDFs; 2. bind to the Ah-receptor; 3. elicit an Ah-receptor mediated biochemical and toxic response; and 4. are persistent and accumulate in the food chain (Van den Berg *et al.* 1998; Birnbaum & DeVito 1995).

Van den Berg *et al.* (1998) presents TEF values for use in deriving TEQs for mammals, fish and birds. These TEFs are listed in Table 1.

Table 1. TEF values presented in Van den Berg *et al.* 1998 for mammals, fish, and birds.

No.	Congener	Mammals	Fish	Birds
		TEF		
1	PCB-77	0.0001	0.0001	0.05
2	PCB-81	0.0001	0.0005	0.1
3	PCB-126	0.1	0.005	0.1
4	PCB-169	0.01	0.00005	0.001
5	PCB-105	0.0001	<0.000005[1]	0.0001
6	PCB-114	0.0005	<0.000005[1]	0.0001
7	PCB-118	0.0001	<0.000005[1]	0.00001
8	PCB-123	0.0001	<0.000005[1]	0.00001
9	PCB-156	0.0005	<0.000005[1]	0.0001
10	PCB-157	0.0005	<0.000005[1]	0.0001
11	PCB-167	0.00001	<0.000005[1]	0.00001
12	PCB-189	0.0001	<0.000005[1]	0.00001
13	1,2,3,4,6,7,8-HPCDD	0.01	0.001	<0.001[1]
14	1,2,3,4,6,7,8-HPCDF	0.01	0.01	0.01
15	1,2,3,4,7,8,9-HPCDF	0.01	0.01	0.01
16	1,2,3,4,7,8-HXCDD	0.1	0.5	0.05
17	1,2,3,4,7,8-HXCDF	0.1	0.1	0.1
18	1,2,3,6,7,8-HXCDD	0.1	0.01	0.01
19	1,2,3,6,7,8-HXCDF	0.1	0.1	0.1
20	1,2,3,7,8,9-HXCDD	0.1	0.01	0.1
21	1,2,3,7,8,9-HXCDF	0.1	0.1	0.1
22	1,2,3,7,8-PECDD	1	1	1
23	1,2,3,7,8-PECDF	0.05	0.05	0.1
24	2,3,4,6,7,8-HXCDF	0.1	0.1	0.1
25	2,3,4,7,8-PECDF	0.5	0.5	1
26	2,3,7,8-TCDD	1	1	1
27	2,3,7,8-TCDF	0.1	0.05	1
28	OCDD	0.0001	<0.0001[1]	0.0001
29	OCDF	0.0001	<0.001[1]	0.0001

[1] Values that are less than should be considered to be the upper limit for use in any TEQ calculation

TEQs for Housatonic Tissue Data

To derive TEQ values for tissue data, all 29 congeners found in Table 1 must have been analysed for and reported as separate results. A review of the data in the Housatonic tissue database has shown that the tissue samples do not have all 29 congeners individually reported. Two of the target 29 congeners co-elute. PCB-157 and PCB-123 were reported as part of a triplet (PCB-201/**157**/173) and doublet (PCB-149/**123**) respectively, in the GERG analytical method. PCB-123 and PCB-157 are relatively small constituents of the technical Aroclor mixtures 1254 and 1260 (Table 2). The majority of the tissue data analysis results present in the database has been performed in accordance with the GERG statement of protocol (SOP). The protocol used by GERG for analyzing tissue data are described in the "Quality Assurance Project Plan (QAPP) Addendum for Tissue Analysis" (DCN: GEP2-060499-AAIY).

Table 2. Weight (%) of co-eluted congeners found in technical mixtures of Aroclor-1254 and Aroclor-1260 (Frame *et al.*)

PCB Congener	Aroclor Composition (Weight %)		
	Aroclor 1254a	Aroclor 1254g	Aroclor 1260
PCB-123	0.15	0.32	0
PCB-149	3.65	1.82	8.75
PCB-157	0.19	0.30	0.02
PCB-173	0	0	0.1
PCB-201	0	0	0.24

There is a separate database available that contains tissue data provided by GE. The GE data have not been considered in this analysis. The reason for this is simply that the available GE tissue data currently in the database reports only Aroclor values rather than congener values. Thus, it is not possible to derive a TEQ using these data. GE does provide data with congener analysis with samples taken in the Housatonic River in the state of Connecticut; however, this paper is limited to data from the Housatonic primary study area in Massachusetts from the confluence to Wood's Pond.

Two different values for three congeners are reported in Aroclor 1254 as measurements were made in two different lots of the same Aroclor (*i.e.*, Lot a and Lot g). Coliano (1998) reported that substantial differences in Aroclor lot-to-lot congener ratios (for Aroclor 1254 and 1248) are often found due to numerous 4-6 chlorine congeners being created and altered during the aroclor manufacturing process. Degradation and other processes (*e.g.*, preferential bioaccumulation, chemical transformation) can cause large changes in the congener proportions detected in an environmental sample versus those found in the technical mixtures (Cogliano 1998). In a previous analysis (Appendix 3), the relative contributions of PCB-123/149 and PCB-201/157/173 to TEQ calculations were estimated. This analysis assumed that the whole triplet (PCB-201/157/173) and doublet (PCB-149/123) were PCB-157 and PCB-123, respectively. The two congeners (PCB-123 & PCB-157) were found to comprise up to 54% or as little as 8% of the total maximum TEQ. The majority of the results showed an approximately 33% contribution of the congeners to the TEQ. These contributions are substantial and must be addressed in any future TEQ calculations for the ERA.

ISSUE RESOLUTION

Fish

Dr. Don Tillitt, Biochemistry & Physiology Branch, Columbia Environmental Research Center, United States Geological Survey (USGS) has analyzed fish tissue samples from the Housatonic River for use in the largemouth bass reproduction study. The fish are largemouth bass (*Micropterus salmoides*) and were sampled from different locations along the Housatonic River in 1999. The analytical protocol used to determine PCB congeners in the fish varied from the one used by GERG in that multiple extraction columns with carbon enrichment were used. The extra steps aid in the elution process and provide better resolution of the individual congeners. Three fish were sampled from each of Rising Pond, Wood's Pond, Deep Reach Pond and Three Mile Pond. Table 3 summarizes this data set (Tillitt, personnal communication of 1999 data from H.R.). From the data in Table 3, the relative proportion of each of the congeners that make up the doublet and triplet in the Housatonic data was determined for the largemouth bass data (Tillitt, *per. comm.*, June 25, 2001).

Table 3. Largemouth bass tissue data (Tillitt personnal communication, June 25, 2001 -data from H.R.) and ratios of PCB congeners that comprise the doublet (PCB-123/149) and triplet (PCB-201/157/173).

	Concentration (ng/g)						Proportion				
Sample ID	PCB 123	PCB 149	PCB 157	PCB 173	PCB 201		123 123/149	149 123/149	157 201/157/173	201 201/157/173	173 201/157/173
RP-A	13	2,600	34	14	67		0.0051	0.995	0.298	0.580	0.122
RP-B	13	2,700	36	14	69		0.0048	0.995	0.301	0.580	0.119
RP-C	12	2,400	33	13	61		0.0049	0.995	0.307	0.569	0.124
Average	13	2,600	34	14	66		0.0049	0.995	0.302	0.576	0.122
SD(n-1)	0.73	153	1.6	0.53	4.4						
CV	6	6	5	4	7						
WP-A	18	6,400	56	63	240		0.0028	0.997	0.157	0.669	0.174
WP-B	24	8,700	75	98	330		0.0027	0.997	0.149	0.656	0.195
WP-C	20	6,300	54	77	250		0.0032	0.997	0.142	0.656	0.202
Mean	20	7,100	62	79	270		0.0029	0.997	0.149	0.660	0.190
SD(n-1)	3.0	1,400	11	18	49						
CV	15	20	18	23	18						
DRP-A	21	9,500	63	120	400		0.0022	0.998	0.108	0.686	0.206
DRP-B	23	11,000	96	130	420		0.0021	0.998	0.148	0.650	0.201
DRP-C	22	10,000	86	130	380		0.0022	0.998	0.144	0.638	0.218
Mean	22	10,000	81	130	400		0.0022	0.998	0.133	0.658	0.208
SD(n-1)	0.6	760	17	6	20						
CV	3	8	21	4	5						
MP3-B**	0.29	50	0.83	0.28	1.3		0.0059	0.994	0.348	0.537	0.115
MP3-C	0.02	2.4	< 0.12	0.04	0.12		0.0080	0.992	-	-	-
MP3-D	< 0.01	2.5	< 0.12	0.03	0.06		-	-	-	-	-
Mean	0.16	18		0.11	0.49		0.0046	-	-	-	-
SD(n-1)	0.19	27		0.1	0.69						
CV	120	150		120	140						
						Mean:	**0.003**	**0.997**	**0.195**	**0.632**	**0.174**
						SD:	**0.0012**	**0.0012**	**0.077**	**0.041**	**0.038**

** - MP3-B is an outlier and is not used in the calculations of the mean for MP3-B
SD – Standard deviation
CV – Coefficient of Variation
WP = Wood's Pond; RP= Rising Pond; DRP = Deep Reach Pond; MP3 = Three Mile Pond

The ratios for PCB-123 and PCB-157 can be used to determine the contribution of these congeners to the doublet and triplet as reported in the Housatonic tissue database. The following calculation (Equation 2) should be performed with the Housatonic River fish tissue data results from GERG.

$$PCB-123_H = PCB-123_T * (PCB-123/149_H) \qquad \textbf{EQ. 2}$$

$$PCB-157_H = PCB-157_T * (PCB-201/157/173_H) \qquad \textbf{EQ. 3}$$

Where,

$PCB\text{-}123_H$ – Concentration of PCB-123 in the Housatonic River fish sample analyzed by GERG
$PCB\text{-}157_H$ – Concentration of PCB-157 in the Housatonic River fish sample analyzed by GERG
$PCB\text{-}123_T$ – Average ratio of PCB-123 in the largemouth bass (Table 4) analyzed by Tillitt and co-workers
$PCB\text{-}157_T$ – Average ratio of PCB-157 in the largemouth bass (Table 4) analyzed by Tillitt and co-workers
$PCB\text{-}123/149_H$ – PCB-123/149 doublet in fish tissue data as reported in Housatonic database
$PCB\text{-}201/157/173_H$ – PCB-201/157/173 in fish tissue data as reported in Housatonic database

The calculations may be done using point estimates as inputs (*e.g.*, for the screening level exposure analysis) or distributions for the inputs (*e.g.*, for probabilistic exposure analyses). To illustrate the application of these calculations to fish data in the Housatonic River, data for a single unique whole body fish were isolated from the tissue database and a TEQ developed (Table 4). In this fish sample, PCB-126 and PCB-118 (both detected values with no qualifiers) are large contributers to the sample TEQ (38% and 19.5%, respectively). The dioxin and furans congeners and PCB-114 (the only non-detected PCB congener) contribute little to the sample TEQ. The co-eluted congeners PCB-123 and PCB-157 had a small contribution to the sample TEQ (3.9%).

Table 4. Polychlorinated hydrocarbon (PCH) data isolated for one unique fish sample (Field Sample ID # H3-TW11GF03-0-8C20) from the Housatonic database and (06/12/01 version) and TEQ calculation results

Congener	Concentration[1] (mg/kg)	Proportion in Co-eluted Sample	Corrected Concentration[5] (mg/kg)	Mammalian TEF (Van den Berg *et al.* 1999)	Congener TEQ	Proportion of Total TEQ
PCB-77	0.005447	NA	NA	0.0001	5.45E-07	6.12E-04
PCB-81	0.000862	NA	NA	0.0001	8.62E-08	9.69E-05
PCB-105	0.463743	NA	NA	0.0001	4.64E-05	5.21E-02
PCB-114	0.0002[2]	NA	NA	0.0005	1.00E-07	1.12E-04
PCB-118	1.728937	NA	NA	0.0001	1.73E-04	1.94E-01
PCB-126	0.003347	NA	NA	0.1	3.35E-04	3.76E-01
PCB-156	0.422	NA	NA	0.0005	2.11E-04	2.37E-01
PCB-167	0.212862	NA	NA	0.00001	2.13E-06	2.39E-03
PCB-169	0.001258	NA	NA	0.01	1.26E-05	1.42E-02
PCB-189	0.029064	NA	NA	0.0001	2.91E-06	3.27E-03
PCB-149/123[3]	**8.269354**	0.003	0.0248	0.0001	2.48E-06	2.79E-03
PCB-201/157/173[4]	**0.329227**	0.195	0.0642	0.0005	3.21E-05	3.61E-02
2,3,7,8-TCDD	0.000002	NA	NA	1	2E-06	2.2E-03
2,3,7,8-TCDF	0.0000126	NA	NA	0.1	1.26E-06	1.42E-03
1,2,3,7,8-PECDD	0.00000313	NA	NA	1	3.13E-06	3.52E-03
1,2,3,7,8,9-HXCDD	0.00000313	NA	NA	0.1	3.13E-07	3.52E-04
1,2,3,6,7,8-HXCDD	0.00000313	NA	NA	0.1	3.13E-07	3.52E-04
1,2,3,4,7,8-HXCDD	0.00000313	NA	NA	0.1	3.13E-07	3.52E-04
OCDF	0.00000627	NA	NA	0.0001	6.27E-10	7.04E-07
OCDD	0.0000109	NA	NA	0.0001	1.09E-09	1.22E-06
1,2,3,7,8-PECDF	0.0007208	NA	NA	0.05	3.60E-05	4.04E-02
2,3,4,7,8-PECDF	0.0000414	NA	NA	0.5	2.07E-05	2.33E-02
1,2,3,4,7,8-HXCDF	0.00000313	NA	NA	0.1	3.13E-07	3.52E-04
1,2,3,6,7,8-HXCDF	0.00000313	NA	NA	0.1	3.13E-07	3.52E-04
2,3,4,6,7,8-HXCDF	0.00000313	NA	NA	0.1	3.13E-07	3.52E-04
1,2,3,7,8,9-HXCDF	0.00000313	NA	NA	0.1	3.13E-07	3.52E-04
1,2,3,4,6,7,8-HPCDF	0.0006509	NA	NA	0.01	6.51E-06	7.31E-03
1,2,3,4,7,8,9-HPCDF	0.00000313	NA	NA	0.01	3.13E-08	3.52E-05
1,2,3,4,6,7,8-HPCDD	0.0000028	NA	NA	0.01	2.80E-08	3.15E-05
				TEQ:	**8.9E-04**	**1**

1 non-detects were assigned a value of half the sample detection limit for this analysis
2 not detected
3 PCB-123 required in TEQ calculation
4 PCB-157 required in TEQ calculation
5 See equations 2 and 3, table 4
NA = Not applicable

An elasticity analysis was performed to determine what the effect of a two fold error on the generated ratios may have on the overall TEQ values. Twenty unique fish samples were examined for this analysis. The results are presented in Table 5 and 6.

Table 5. Results of elasticity analysis of suggested fish tissue ratios assuming the ratios are off by a factor of 2

Field Sample ID	1 x Ratio			2 x Ratio		
	TEQ	Proportion PCB-123	Proportion PCB-157	TEQ	Proportion PCB-123	Proportion PCB-157
H3-TW03FFC1-0-8C02	0.00048	0.00185	0.02366	0.00050	0.00361	0.04613
H3-TW03FFC1-0-8C19	0.00048	0.00108	0.03098	0.00049	0.00210	0.06003
H3-TW03FFC2-0-8C02	0.00033	0.00254	0.03139	0.00034	0.00492	0.06071
H3-TW03FFC2-0-8C19	0.00049	0.00179	0.03368	0.00051	0.00346	0.06505
H3-TW03FFC3-0-8C19	0.00064	0.00161	0.02555	0.00066	0.00313	0.04975
H3-TW03LB01-0-8C19	0.00015	0.00089	0.01403	0.00015	0.00176	0.02764
H3-TW03LB02-0-8C19	0.00183	0.00195	0.03353	0.00189	0.00376	0.06477
H3-TW03LB03-0-8C20	0.00021	0.00079	0.01414	0.00021	0.00156	0.02787
H3-TW03LB04-0-8C20	0.00177	0.00217	0.03628	0.00184	0.00419	0.06987
H3-TW03LB05-0-8C20	0.00006	0.00074	0.01591	0.00006	0.00145	0.03129
H3-TW03LBC1-0-8C02	0.00052	0.00140	0.01479	0.00053	0.00276	0.02911
H3-TW03LBC2-0-8C02	0.00096	0.00086	0.01351	0.00097	0.00170	0.02663
H3-TW03SB01-0-8C20	0.00130	0.00155	0.02727	0.00134	0.00302	0.05302
H3-TW03SB02-0-8C20	0.00215	0.00156	0.02890	0.00221	0.00303	0.05609
H3-TW03YPC1-0-8C20	0.00045	0.00080	0.01185	0.00045	0.00159	0.02339
H3-TW03YPC2-0-8C20	0.00039	0.00116	0.00922	0.00039	0.00230	0.01825
H3-TW03YPC3-0-8C20	0.00039	0.00117	0.03080	0.00040	0.00226	0.05970
H3-TW03YPC4-0-8C20	0.00025	0.00112	0.02088	0.00026	0.00219	0.04086
H3-TW03YPC5-0-8C20	0.00067	0.00086	0.01807	0.00068	0.00170	0.03546
H3-TW07GSC1-0-8S30	0.00043	0.00091	0.00851	0.00044	0.00180	0.01686
H3-TW07LB03-0-8S29	0.00103	0.00167	0.02145	0.00105	0.00326	0.04193
H3-TW07LB04-0-8S29	0.00054	0.00189	0.01488	0.00055	0.00371	0.02926
H3-TW07LBC1-0-8S30	0.00041	0.00161	0.01331	0.00042	0.00318	0.02623
H3-TW07PSC1-0-8S29	0.00033	0.00150	0.01648	0.00034	0.00294	0.03237
H3-TW07YPC1-0-8S29	0.00077	0.00074	0.00891	0.00078	0.00147	0.01764
H3-TW03FFC1-0-8C02	0.00048	0.00185	0.02366	0.00050	0.00361	0.04613

Proportion is the proportion of each of the two congeners (PCB-123 and PCB-157) in the generated TEQ at each ratio factor.

Table 6 demonstrates that assuming a 2 x increase in the value of the calculated ratio's for PCB-123 (*i.e.*, 0.003 to 0.006) and PCB-157 (*i.e.*, 0.195 to 0.39), the final TEQ is sensitive to changes in the calculated ratios. For the twenty samples examined, the two fold increase in the value of the two ratio's resulted in an increase in the TEQ ranging from 0% to 4% for the twenty tested samples.

Table 6. Difference in TEQ values assuming a 2X and 10X increase in the calculated fish tissue ratio's

Field Sample ID	TEQ 1 X	TEQ 2 X	Difference (TEQ1X – TEQ 2X)
H3-TW03FFC1-0-8C02	0.00048	0.00050	0.00001
H3-TW03FFC1-0-8C19	0.00048	0.00049	0.00002
H3-TW03FFC2-0-8C02	0.00033	0.00034	0.00001
H3-TW03FFC2-0-8C19	0.00049	0.00051	0.00002
H3-TW03FFC3-0-8C19	0.00064	0.00066	0.00002
H3-TW03LB01-0-8C19	0.00015	0.00015	0.00000
H3-TW03LB02-0-8C19	0.00183	0.00189	0.00006
H3-TW03LB03-0-8C20	0.00021	0.00021	0.00000
H3-TW03LB04-0-8C20	0.00177	0.00184	0.00007
H3-TW03LB05-0-8C20	0.00006	0.00006	0.00000
H3-TW03LBC1-0-8C02	0.00052	0.00053	0.00001
H3-TW03LBC2-0-8C02	0.00096	0.00097	0.00001
H3-TW03SB01-0-8C20	0.00130	0.00134	0.00004
H3-TW03SB02-0-8C20	0.00215	0.00221	0.00007
H3-TW03YPC1-0-8C20	0.00045	0.00045	0.00001
H3-TW03YPC2-0-8C20	0.00039	0.00039	0.00000
H3-TW03YPC3-0-8C20	0.00039	0.00040	0.00001
H3-TW03YPC4-0-8C20	0.00025	0.00026	0.00001
H3-TW03YPC5-0-8C20	0.00067	0.00068	0.00001
H3-TW07GSC1-0-8S30	0.00043	0.00044	0.00000
H3-TW07LB03-0-8S29	0.00103	0.00105	0.00002
H3-TW07LB04-0-8S29	0.00054	0.00055	0.00001
H3-TW07LBC1-0-8S30	0.00041	0.00042	0.00001
H3-TW07PSC1-0-8S29	0.00033	0.00034	0.00001

Uncertainty

There are several sources of uncertainty associated with the method for treating the co-eluted congeners. The first is interlaboratory variance due to different analytical methods, laboratory conditions, and analyst practices and expertise (*i.e.*, GERG and USGS). The calculated ratios also do not account for differences between species found in the tissue database. Only data for largemouth bass were found that could be used to calculate the ratios. These ratios could differ due to different metabolization rates of some congeners amongst fish species. However, we assume that due to the fact that the fish species sampled from the Housatonic are all warm-water, freshwater species, the different metabolism rates of congeners between the fish species sampled is likely not substantial (Tillet, *pers comm.* July 5th, 2001).

Both spatial and temporal uncertainty also may be important. Spatially, the largemouth bass were sampled at four sites along the river (three of which were used in the calculations) (*i.e.*, Wood's Pond, Rising Pond, and Deep Reach Pond). The Three Mile Pond (MP3) data were not used as the doublet and triplet congeners were detected below the detection limit in two samples and one (*i.e.*, MP3-B) was determined to be an outlier.

Spatial variability could be taken into account by fitting distributions to the sample ratios calculated for PCB-123 and PCB-157. Temporally, the two congeners in the doublet (PCB-123/149) and the three congeners in the triplet (PCB-201/157/173) co-eluted. This indicates that they have very similar structures (*i.e.*, part of the reason that they were co-eluted). Therefore, they may have similar fate and behaviour in the environment. However, due to the small number of samples used to generate the ratios and the single sampling time (*i.e.*, 1999), it is difficult to address this source of uncertainty in the current analysis.

Mammals, Birds, Invertebrates, Amphibians, Vegetation

There are no data currently available for mammals, birds, amphibians, vegetation, and invertebrates that can be used to derive congener ratios for use with the GERG data. The applicability of the congener ratios developed using largemouth bass samples to other tissue samples (*e.g.*, mammal, bird and invertebrate) is unknown. The authors are currently considering the worldwide literature to determine if congener ratios can be developed for PCB-123 and PCB-157 for mammals, birds and invertebrates. Alternatively, these tissue samples could be collected from the Housatonic River and submitted to Dr. Don Tillitt's laboratory for congeners analysis. A key factor that must be addressed particularly for mammals and birds is the rate at which different species metabolize the congeners. Boon *et al.* (1997) demonstrated that for different fish eating mammals (*e.g.*, otter, dolphin, seals), there were substantial differences in the ability of these mammals to metabolize PCB congeners. Development of ratio's to address the co-elution of congeners, as done for fish above, would therefore be difficult without addressing the rate of metabolism of specific congeners for each species.

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APPENDICES

Appendix 1. Congener composition data for Aroclors 1254 and 1260 (Frame *et al.* 1996)

BZ/IUPAC Number	Chlorine Substitution Pattern (IUAPC)	Aroclor Composition (Wt %)		
		1254g	1254a	1260
1	2	0.02		0.02
4	2,2'	0.02	0.06	0.02
6	2,3'	0.01	0.02	0.01
8	2,4'	0.05	0.13	0.04
15	4,4'	0.01	0.03	0.01
16	2,2',3	0.02	0.09	0.01
17	2,2',4	0.02	0.08	0.02
18	2,2'5	0.08	0.25	0.05
22	2,3,4'	0.02	0.04	0.01
26	2,3',5		0.03	
28	2,4,4'	0.06	0.19	0.03
31	2,4',5	0.11	0.28	0.04
32	2,4',6	0.01	0.05	0.01
33	2,3',4'	0.05	0.16	0.03
37	3,4,4'	0.01	0.07	0.01
40	2,2',3,3'	0.15	0.12	
41	2,2',3,4	0.02	0.01	
42	2,2',3,4'	0.09	0.15	0.01
44	2,2',3,5'	0.67	2.31	0.03
45	2,2',3,6	0.02	0.05	
47	2,2',4,4'	0.07	0.14	
48	2,2',4,5	0.05	0.12	
49	2,2',4,5'	0.26	1.10	0.01
52	2,2',5,5'	0.83	5.38	0.24
53	2,2',5,6'	0.04	0.12	
56	2,3,3',4'	1.70	0.55	0.02
59	2,3,3',6	0.01	0.02	
60	2,3,4,4'	0.95	0.18	0.04
63	2,3,4',5	0.07	0.02	
64	2,3,4',6	0.36	0.59	0.01
66	2,3',4,4'	3.56	1.01	0.02
67	2,3',4,5	0.01		
70	2,3',4',5	6.83	3.49	0.04
71	2,3',4',6	0.11	0.15	0.01
74	2,4,4',5	2.19	0.84	0.05
76	2,3',4',5'	0.03	0.02	
77	3,3',4,4'	0.20	0.03	
81	3,4,4',5	trace		
82	2,2'3,3',4	1.53	1.11	
83	2,2,3,3',5	0.56	0.48	0.01
84	2,2,',3,3',6	1.58	2.32	0.11

BZ/IUPAC Number	Chlorine Substitution Pattern (IUAPC)	Aroclor Composition (Wt %)		
		1254g	1254a	1260
85	2,2',3,4,4'	2.49	1.28	0.01
86	2,2',3,4,5	0.10	0.06	
87	2,2',3,4,5'	3.41	3.99	0.41
89	2,2',3,4,6'	0.11	0.09	
90	2,2',3,4',5	nm/bp	nm/bp	
91	2,2',3,4',6	0.53	0.93	0.01
92	2,2',3,5,5'	0.57	1.29	0.30
94	2,2',3,5,6'	0.01	0.02	
95	2,2',3,5',6	1.84	6.25	2.45
96	2,2',3,6,6'	0.01	0.04	
97	2,2',3,4',5'	2.78	2.62	0.09
99	2,2',4,4',5	4.53	3.02	0.04
101	2,2'4,5,5'	5.49	8.02	3.13
102	2,2',4,5,6'	0.09	0.15	
103	2,2',4,5',6		0.03	
105	2,3,3',4,4'	7.37	2.99	0.22
107	2,3,3',4',5	0.78	0.37	0.01
110	2,3,3',4',6	8.42	9.29	1.33
113	2,3,3',5',6	0.01		
114	2,3,4,4',5	0.50	0.18	
115	2,3,4,4',6	0.37	0.20	
117	2,3,4',5,6	0.19	0.23	
118	2,3'4,4',5	13.59	7.35	0.48
119	2,3',4,4',6	0.12	0.08	
122	2,3,3',4',5'	0.25	0.10	
123	2,3',4,4',5'	0.32	0.15	
124	2,3',4',5,5'	0.47	0.29	0.01
125	2,3',4',5',6	0.03	0.02	
126	3,3',4,4',5	0.02	trace	
128	2,2',3,3',4,4'	1.71	1.42	0.53
129	2,2',3,3',4,5	0.39	0.38	0.14
130	2,2',3,3',4,5'	0.50	0.60	0.22
131	2,2',3,3',4,6	0.14	0.19	0.07
132	2,2',3,3',4,6'	1.50	2.29	2.90
133	2,2',3,3',5,5'		0.11	0.07
134	2,2',3,3',5,6	0.20	0.37	0.34
135	2,2',3,3',5,6'	0.28	0.61	1.08
136	2,2'3,3',6,6'	0.24	0.70	1.46
137	2,2',3,4,4',5	0.52	0.42	0.02
138	2,2',3,4,4',5'	5.95	5.80	6.54
139	2,2',3,4,4',6	0.14	0.15	
141	2,2',3,4,5,5'	0.69	0.98	2.62
144	2,2',3,4,5',6	0.12	0.24	0.61

BZ/IUPAC Number	Chlorine Substitution Pattern (IUAPC)	Aroclor Composition (Wt %)		
		1254g	1254a	1260
146	2,2',3,4',5,5'	0.45	0.67	1.15
147	2,2',3,4',5,6	0.02	0.10	
149	2,2',3,4',5',6	1.82	3.65	8.75
151	2,2',3,5,5',6	0.22	0.69	3.04
153	2,2',4,4',5,5'	3.29	3.77	9.39
154	2,2',4,4',5,6'	0.02	0.04	
156	2,3,3',4,4',5	1.13	0.82	0.52
157	2,3,3',4,4',5'	0.30	0.19	0.02
158	2,3,3',4,4',6	0.90	0.81	0.58
163	2,3,3',4',5,6	0.70	1.03	2.42
164	2,3,3',4',5',6	0.31	0.40	0.69
166	2,3,4,4',5,6	0.05	0.05	
167	2,3',4,4',5,5'	0.35	0.27	0.19
170	2,2',3,3',4,4',5	0.35	0.52	4.11
171	2,2',3,3',4,4',6	0.08	0.14	1.11
172	2,2',3,3',4,5,5'	0.03	0.07	0.70
173	2,2',3,3',4,5,6			0.10
174	2,2',3,3',4,5,6'	0.14	0.34	4.96
175	2,2',3,3',4,5',6			0.17
176	2,2',3,3',4,6,6'	0.01	0.04	0.59
177	2,2',3,3',4,5',6'	0.08	0.20	2.57
178	2,2',3,3',5,5',6		0.03	0.83
179	2,2',3,3',5,6,6'	0.02	0.10	2.03
180	2,2',3,4,4',5,5'	0.42	0.67	11.38
181	2,2',3,4,4',5,6			0.01
183	2,2',3,4,4',5',6	0.09	0.18	2.41
185	2,2',3,4,5,5',6			0.55
187	2,2',3,4',5,5',6	0.09	0.25	5.40
189	2,3,3',4,4',5,5'	0.01	0.01	0.10
190	2,3,3',4,4',5,6	0.05	0.07	0.82
191	2,3,3',4,4',5,6			0.17
193	2,3,3',4',5,5',6		0.03	0.53
194	2,2',3,3',4,4',5,5'		0.01	2.07
195	2,2',3,3',4,4',5,6			0.84
196	2,2',3,3',4,4',5,6'			1.09
197	2,2',3,3',4,4',6,6'			0.07
198	2,2',3,3',4,5,5',6			0.10
199	2,2',3,3',4,5,5',6'		0.01	1.78
200	2,2',3,3',4,5,6,6'			0.25
201	2,2',3,3',4,5',6,6'			0.24
202	2,2',3,3',5,5',6,6'			0.33
203	2,2',3,4,4',5,5',6		0.02	1.40
205	2,3,3',4,4',5,5',6			0.10

BZ/IUPAC Number	Chlorine Substitution Pattern (IUAPC)	Aroclor Composition (Wt %)		
		1254g	1254a	1260
206	2,2',3,3',4,4',5,5',6	0.03	0.03	0.53
207	2,2',3,3',4,4',5,6,6'			0.05
208	2,2',3,3',4,5,5',6,6'	0.01	0.01	0.13
209	2,2',3,3',4,4',5,5',6,6'			nm/bp

Notes:

Blank spaces are non-detects, congeners not included are also non-detects.

"trace" refers to samples above the detection limit, but below the level of quantitation (0.01%).

"nm/bp" represents congeners that were not measured due to method limitations, but are believed to exist as a result of past studies.

The "a" and "g" on the 1254 congeners represent the Lots where the samples were taken.

Appendix 2. SQL Queries designed to isolate Housatonic River tissue data for fish, apply the TEF, and calculate the TEQ.

The first query (SQL1) "Fish Query" isolates fish data from the Housatonic river between the confluence and including Wood's Pond using the FACILITY_ID field H3 / H4. Whole body data are used (*i.e.*, mink don't eat just ovaries) and is isolated using Tissue_Sample_Type = "WH", "IN", "CM. The code WH is defined as whole body, IN means individual, and CM is composite. IN could refer either to individual fish or individual body parts. CM means a composite sample of small whole body fish. There will be some ovary data in this Fish query that can be eliminated before continuing. Only data that have a QC Level of 2, 5, 10, and 11 are used.

NOTE: *THINGS TO WATCH FOR WHEN DOING THIS TYPE OF CALCULATION*

1. Always make certain that each unique sample ID has all of the congeners required to calculate a TEQ. If it is missing one congener the TEQ estimate will be incorrect. It may be possible to justify why that particular congener is not important (*e.g.*, makes up only a very insignificant portion of the TEQ) and be able to use it in any further analysis.

2. Watch how non-detects are treated. The queries below give you the option of using a non-detect value of 0 or taking half the detection limit (DL) (*i.e.*, 0 or DL/2)

3. Make sure to use the correct TEFs. For example, mink as predator means the mammalian TEFs are used. Birds as predator means the bird TEFs are used,etc. There are no TEFs for invertebrates as predator.

4. Watch for co-eluted congeners.

5. Make certain that when isolating the data to use the appropriate tissue type (*e.g.*, whole body vs. ovaries)

6. Make certain to use the appropriate TEFs for the calculations. The Eco-Risk side of the project is using the Van den Berg *et al.* (1999) TEFs of which there are three possibilities: Mammals as predator, Birds as predator, and Fish as predator.

SQL1 (Fish Query)--

```
SELECT FIN_DM_TISSUE.LAB_CODE, FIN_DM_TISSUE.COLLECTED_DATE,
FIN_DM_TISSUE.FACILITY_ID, FIN_DM_TISSUE.TISSUE_SPECIES,
FIN_DM_TISSUE.LOCATION_TYPE, FIN_DM_TISSUE.FIELD_SAMPLE_ID,
FIN_DM_TISSUE.TISSUE_SAMPLE_TYPE, FIN_DM_TISSUE.SPECIMEN_LENGTH,
FIN_DM_TISSUE.TISSUE_NUM_IN_COMP,
FIN_DM_TISSUE.TISSUE_AVG_LENGTH_IN_COMPOSITE,
FIN_DM_TISSUE.TISSUE_BODY_PART, FIN_DM_TISSUE.TISSUE_AGE,
FIN_DM_TISSUE.TISSUE_WEIGHT, FIN_DM_TISSUE.TISSUE_SPECIMEN_WEIGHT,
FIN_DM_TISSUE.COC_CATEGORY, FIN_DM_TISSUE.CAPTION,
FIN_DM_TISSUE.NUM_RES, FIN_DM_TISSUE.RESULT_FLAG,
FIN_DM_TISSUE.RESULT_UNITS, FIN_DM_TISSUE.QC_LEVEL,
FIN_DM_TISSUE.CENTRAL_LOCATION_DESCRIPTION, FIN_DM_TISSUE.X_COORD,
FIN_DM_TISSUE.Y_COORD
FROM FIN_DM_TISSUE
WHERE (((FIN_DM_TISSUE.FACILITY_ID)="H3" Or (FIN_DM_TISSUE.FACILITY_ID)="H4")
AND ((FIN_DM_TISSUE.LOCATION_TYPE)="TF" Or
(FIN_DM_TISSUE.LOCATION_TYPE) Is Null) AND
((FIN_DM_TISSUE.TISSUE_SAMPLE_TYPE)="WH" Or
(FIN_DM_TISSUE.TISSUE_SAMPLE_TYPE)="CM" Or
(FIN_DM_TISSUE.TISSUE_SAMPLE_TYPE)="IN") AND
((FIN_DM_TISSUE.COC_CATEGORY)="PCBS" Or
(FIN_DM_TISSUE.COC_CATEGORY)="PCB CONGENERS" Or
(FIN_DM_TISSUE.COC_CATEGORY)="DIOXINS/FURANS") AND
((FIN_DM_TISSUE.CAPTION) Not Like "AROCLOR*" And
(FIN_DM_TISSUE.CAPTION)<>"PCB, TOTAL") AND
((FIN_DM_TISSUE.RESULT_FLAG)<>"I" Or (FIN_DM_TISSUE.RESULT_FLAG)<>"R" Or
(FIN_DM_TISSUE.RESULT_FLAG) Is Null) AND ((FIN_DM_TISSUE.QC_LEVEL)=2 Or
(FIN_DM_TISSUE.QC_LEVEL)=5 Or (FIN_DM_TISSUE.QC_LEVEL)=10 Or
(FIN_DM_TISSUE.QC_LEVEL)=11));
```

SQL2 (qryFish_TEF)---

```
SELECT [Fish Query].TISSUE_SPECIES, [Fish Query].LOCATION_TYPE, [Fish
Query].FIELD_SAMPLE_ID, [Fish Query].TISSUE_SAMPLE_TYPE, [Fish
Query].SPECIMEN_LENGTH, [Fish Query].TISSUE_NUM_IN_COMP, [Fish
Query].TISSUE_AVG_LENGTH_IN_COMPOSITE, [Fish Query].TISSUE_AGE, [Fish
Query].TISSUE_WEIGHT, [Fish Query].TISSUE_SPECIMEN_WEIGHT, [Fish Query].CAPTION,
[Fish Query].NUM_RES, IIf([RESULT_FLAG]="U" Or
[RESULT_FLAG]="UJ",[NUM_RES]/2,[NUM_RES]) AS NUM_RES_DL, IIf([CAPTION]="PCB-
149/123",[NUM_RES_DL]*0.003,IIf([CAPTION]="PCB-
201/157/173",[NUM_RES_DL]*0.195,[NUM_RES_DL])) AS [Co-elution], [Co-
elution]*[lkpTEF_Mammals2]![WHO TEF] AS TEF_Calc, [Fish Query].RESULT_UNITS, [Fish
Query].RESULT_FLAG, [Fish Query].QC_LEVEL, [Fish
Query].CENTRAL_LOCATION_DESCRIPTION
FROM lkpTEF_Mammals2 INNER JOIN [Fish Query] ON lkpTEF_Mammals2.CONGENER =
[Fish Query].CAPTION;
```

SQL3 (qryFish_TEQ)---

```
SELECT qryFish_TEF.FIELD_SAMPLE_ID, Sum(qryFish_TEF.TEF_Calc) AS SumOfTEF_Calc
FROM qryFish_TEF
GROUP BY qryFish_TEF.FIELD_SAMPLE_ID;
```

Appendix 3. Previous analysis of the Congener co-elution issue including an examination of the impact of co-elution of TEQ calculations.

Database Used: FIN_DM_TISSUE
Database Date: 04/19/01

The Issue

This appendix examines the potential impact of congener PCB-157 and PCB-123 on the Toxic Equivalent Concentrations (TEQ) calculations for fish tissue from the Housatonic River between the confluence to Wood's Pond.

PCB-157 and PCB-123 were reported as part of a triplet (PCB-201/**157**/173) and doublet (PCB-149/**123**), respectively, from the tissue analysis data from GERG. These two congeners are required when calculating TEQ's for Birds, Fish and Mammals using the toxic equivalency factors (TEF) described by Van den Berg *et al.* (1998) (Table A3-1). PCB-123 and PCB-157 are components of Aroclor-1254 and Aroclor-1260 (Frame *et al.* 1996). GE's Transformer Division's activities included the construction and repair of electrical transformers using dielectric fluids, some of which contained PCBs (primarily Aroclors 1254 and 1260).

CONGENER	WHO TEF
PCB-77	0.0001
PCB-81	0.0001
PCB-126	0.1
PCB-169	0.01
PCB-105	0.0001
PCB-114	0.0005
PCB-118	0.0001
PCB-123	**0.0001**
PCB-156	0.0005
PCB-157	**0.0005**
PCB-167	0.00001
PCB-189	0.0001
1,2,3,4,6,7,8-HPCDD	0.01
1,2,3,4,6,7,8-HPCDF	0.01
1,2,3,4,7,8,9-HPCDF	0.01
1,2,3,4,7,8-HXCDD	0.1
1,2,3,4,7,8-HXCDF	0.1
1,2,3,6,7,8-HXCDD	0.1
1,2,3,6,7,8-HXCDF	0.1
1,2,3,7,8,9-HXCDD	0.1
1,2,3,7,8,9-HXCDF	0.1
1,2,3,7,8-PECDD	1
1,2,3,7,8-PECDF	0.05
2,3,4,6,7,8-HXCDF	0.1
2,3,4,7,8-PECDF	0.5
2,3,7,8-TCDF	0.1
OCDD	0.0001
OCDF	0.0001

Table A3-1. Mammalian TEFs from Van den Berg *et al.* 1998.

Issue #1. What are the maximum relative contributions of these two congeners (as the triplet and doublet) to the overall TEQ calculation for fish?

Issue #2. If the results indicate that the contributions are high, what would be the appropriate course of action when calculating TEQs.

DATA QUERY DESIGN AND CALCULATIONS

Fish tissue data for whole body fish (reported in the database as WH, CM and IN where composites were comprised of multiple small <4cm whole body fish) were isolated for the Housatonic River from the confluence to Woods pond. Only data meeting minimum quality control levels were used (see Table A3-2 for the codes generally used to isolate the data. The results yielded 129 unique Field_Sample_IDs for which there were sufficient data to calculate the TEQ for only 100 fish samples (the remaining 29 were missing dioxin and furan congeners).

There are numerous congeners, particularly dioxin and furan congeners that are non-detects. For the purposes of this analysis, these data were identified using the Results_Flag field (U and UJ codes) and the reported value was divided by 2 (*i.e.,* half the analytical detection limit) for use in the TEQ calculations.

(Note: There are 7 SQL statements plus 2 lookup tables for the full analysis please contact Scott Teed if you wish to obtain the queries).

Table A3-2. Fields and criteria used to isolate fish tissue data in the FIN_DM_TISSUE database

Field	Criteria
	Tissue
Lab_ID	US_COE
Facility ID	H3 or H4
TISSUE_SPECIES	None
Location Type	TF
COC Matrix	None
Field Sample ID	None
Tissue Sample Type	WH or CM or IN
Collected Date	None
COC Category	None
Caption	None
Num Res	None
Result Flag	<>"I" Or <>"R" Or Is Null
Result Unit	None
Stat Res	None
QC Level	*2, 5, 10, or 11*
X Coord	None
Y Coord	None
RM X100	None

Results

The results (Table A3-3) show that the calculated TEQ could vary substantially depending upon the assumption used. Maximum TEQ (MAX_TEQ) values that assume the whole triplet and doublet are PCB-123 or PCB-157, respectively, can comprise up to 8 to 54% of the total TEQ. The majority of results show a 33% contribution of these two congeners to the maximum TEQ. Assuming that PCB-123 and PCB-157 are zero causes the minimum TEQ (MIN_TEQ) to be up to two times (2X) lower than the calculated maximum TEQ (Table A3-3). Because the two congeners are a component of the two most commonly detected Aroclors in the river, they should not be removed from the TEQ calculations.

Table A3-3. Results of the analysis of contributions of the doublet and triplet to TEQ calculations for fish tissue. Mammalian TEFs from Van den Berg *et al.* (1999) were used.

FIELD_SAMPLE_ID	MAX_TEQ	MIN_TEQ	DIFFERENCE (MAX-MIN)	RATIO (MAX/MIN TEQ)
H3-TW11GF03-0-8C20	0.0018	0.0009	0.0010	2.166
H4-TWWPGF09-0-8C01	0.0022	0.0010	0.0012	2.116
H3-TW11GF01-0-8C19	0.0013	0.0006	0.0007	2.088
H3-TW03FFC2-0-8C02	0.0006	0.0003	0.0003	2.045
H4-TWWPGF08-0-8C01	0.0023	0.0011	0.0012	2.036
H3-TW09YPC1-0-8S30	0.0004	0.0002	0.0002	1.952
H4-TWWPGF06-0-8C01	0.0014	0.0007	0.0007	1.952
H3-TW11GF01-0-8S30	0.0025	0.0013	0.0012	1.950
H3-TW03LB04-0-8C20	0.0033	0.0017	0.0016	1.947
H3-TW08GF01-0-8S30	0.0076	0.0040	0.0036	1.887
H3-TW03LB02-0-8C19	0.0033	0.0018	0.0015	1.851
H3-TW11GF04-0-8C20	0.0015	0.0008	0.0007	1.834
H3-TW11GF12-0-8C20	0.0026	0.0014	0.0012	1.823
H3-TW03FFC2-0-8C19	0.0008	0.0005	0.0004	1.797
H3-TW11GF05-0-8C20	0.0024	0.0013	0.0010	1.790
H3-TW03FFC1-0-8C02	0.0008	0.0005	0.0004	1.758
H3-TW11GF13-0-8C20	0.0022	0.0012	0.0009	1.745
H3-TW07LB04-0-8S29	0.0009	0.0005	0.0004	1.717
H3-TW11GF02-0-8S30	0.0006	0.0003	0.0002	1.713
H3-TW09LB13-0-8S30	0.0004	0.0002	0.0001	1.711
H4-TWWPGF01-0-8C21	0.0038	0.0022	0.0015	1.690
H4-TWWPGF06-0-8C21	0.0014	0.0008	0.0006	1.689
H3-TW03SB02-0-8C20	0.0035	0.0021	0.0014	1.689
H3-TW03FFC3-0-8C19	0.0011	0.0006	0.0004	1.686
H4-TWWPGF05-0-8C21	0.0043	0.0025	0.0017	1.680
H3-TW03SB01-0-8C20	0.0021	0.0013	0.0009	1.677
H4-TWWPGF19-0-8C01	0.0033	0.0019	0.0013	1.673
H3-TW11GF11-0-8C20	0.0040	0.0024	0.0016	1.668
H4-TWWPLB10-0-8C01	0.0005	0.0003	0.0002	1.666
H4-TVWPLB09-0-9Y13	0.0020	0.0012	0.0008	1.656
H3-TW10YPC1-0-8S30	0.0003	0.0002	0.0001	1.641
H4-TWWPGSC1-0-8C01	0.0004	0.0003	0.0002	1.637
H3-TW08YPC1-0-8S29	0.0005	0.0003	0.0002	1.636
H4-TWWPLBC4-0-8C01	0.0004	0.0003	0.0002	1.629
H4-TWWPYPC1-0-8C01	0.0005	0.0003	0.0002	1.628

FIELD_SAMPLE_ID	MAX_TEQ	MIN_TEQ	DIFFERENCE (MAX-MIN)	RATIO (MAX/MIN TEQ)
H4-TWWPLB18-0-8C01	0.0008	0.0005	0.0003	1.619
H3-TW07LBC1-0-8S30	0.0007	0.0004	0.0003	1.615
H3-TW07PSC1-0-8S29	0.0005	0.0003	0.0002	1.594
H4-TWWPYPC2-0-8C01	0.0005	0.0003	0.0002	1.579
H3-TW11GF04-0-8S30	0.0020	0.0012	0.0007	1.570
H3-TW03YPC3-0-8C20	0.0006	0.0004	0.0002	1.565
H3-TW08LBC1-0-8S30	0.0006	0.0004	0.0002	1.562
H3-TW08GSC1-0-8S30	0.0004	0.0003	0.0002	1.560
H3-TW03LBC1-0-8C02	0.0008	0.0005	0.0003	1.553
H3-TW11GF09-0-8C20	0.0018	0.0012	0.0006	1.551
H4-TWWPGSC5-0-8C01	0.0004	0.0003	0.0001	1.539
H3-TW03FFC1-0-8C19	0.0007	0.0005	0.0002	1.537
H4-TWWPGF12-0-8C01	0.0033	0.0022	0.0011	1.524
H4-TWWPGF13-0-8C01	0.0022	0.0014	0.0007	1.520
H4-TWWPLB25-0-8C01	0.0012	0.0008	0.0004	1.513
H3-TW09LBC1-0-8S30	0.0007	0.0005	0.0002	1.513
H3-TW11GF03-0-8S30	0.0005	0.0003	0.0002	1.511
H4-TWWPPSC3-0-8C21	0.0006	0.0004	0.0002	1.507
H4-TWWPLBC5-0-8C01	0.0004	0.0002	0.0001	1.507
H4-TWWPGF02-0-8C21	0.0024	0.0016	0.0008	1.503
H4-TWWPGF03-0-8C21	0.0014	0.0009	0.0005	1.500
H4-TWWPGF14-0-8C01	0.0022	0.0015	0.0007	1.499
H3-TW03YPC4-0-8C20	0.0004	0.0002	0.0001	1.491
H4-TWWPGSC2-0-8C01	0.0004	0.0003	0.0001	1.478
H3-TW09GSC1-0-8S30	0.0004	0.0003	0.0001	1.477
H3-TW11PSC4-0-8S30	0.0003	0.0002	0.0001	1.473
H3-TW11PSC3-0-8S30	0.0004	0.0002	0.0001	1.449
H4-TWWPGF16-0-8C01	0.0057	0.0039	0.0017	1.443
H3-TW03YPC2-0-8C20	0.0006	0.0004	0.0002	1.440
H4-TWWPGSC3-0-8C01	0.0004	0.0003	0.0001	1.434
H3-TW11PSC2-0-8S30	0.0003	0.0002	0.0001	1.425
H4-TWWPGSC4-0-8C01	0.0004	0.0003	0.0001	1.423
H4-TWWPPSC1-0-8C21	0.0005	0.0004	0.0002	1.405
H3-TW11PSC1-0-8S30	0.0004	0.0003	0.0001	1.402
H3-TW11LB25-0-8S30	0.0012	0.0009	0.0003	1.402
H3-TW03YPC5-0-8C20	0.0009	0.0007	0.0003	1.388
H3-TW11YPC1-0-8S30	0.0003	0.0002	0.0001	1.387

FIELD_SAMPLE_ID	MAX_TEQ	MIN_TEQ	DIFFERENCE (MAX-MIN)	RATIO (MAX/MIN TEQ)
H3-TW11GF10-0-8C20	0.0008	0.0006	0.0002	1.385
H3-TW11LBC1-0-8S30	0.0003	0.0003	0.0001	1.382
H3-TW11GF08-0-8C20	0.0012	0.0009	0.0003	1.377
H3-TW03LB01-0-8C19	0.0002	0.0001	0.0001	1.375
H3-TW08LB06-0-8S30	0.0007	0.0005	0.0002	1.364
H3-TW03LBC2-0-8C02	0.0013	0.0009	0.0003	1.361
H4-TWWPPSC2-0-8C21	0.0007	0.0005	0.0002	1.357
H3-TW11BB06-0-8S30	0.0003	0.0003	0.0001	1.357
H3-TW07GSC1-0-8S30	0.0006	0.0004	0.0001	1.350
H3-TW11LBC2-0-8S30	0.0004	0.0003	0.0001	1.344
H3-TW03LB03-0-8C20	0.0003	0.0002	0.0001	1.342
H3-TW11LB26-0-8S30	0.0004	0.0003	0.0001	1.336
H3-TW03YPC1-0-8C20	0.0006	0.0004	0.0001	1.333
H3-TW03LB05-0-8C20	0.0001	0.0001	0.0000	1.333
H4-TWWPYPC4-0-8C01	0.0004	0.0003	0.0001	1.316
H3-TW07YPC1-0-8S29	0.0010	0.0008	0.0002	1.295
H4-TWWPYPC5-0-8C01	0.0004	0.0003	0.0001	1.284
H4-TWWPYPC3-0-8C01	0.0004	0.0003	0.0001	1.284
H4-TWWPPSC2-0-8C01	0.0004	0.0003	0.0001	1.282
H4-TWWPLBC1-0-8S30	0.0005	0.0004	0.0001	1.192
H4-TWWPLB26-0-8C01	0.0006	0.0005	0.0001	1.191
H4-TWWPLBC3-0-8S30	0.0003	0.0003	0.0001	1.174
H4-TWWPLB09-0-8C01	0.0003	0.0003	0.0000	1.165
H4-TWWPLBC2-0-8S30	0.0005	0.0004	0.0001	1.148
H4-TWWPPSC1-0-8S30	0.0004	0.0003	0.0000	1.139
3-TW11GSC1-0-8S30	0.0004	0.0004	0.0000	1.128
H4-TWWPGF04-0-8C01	0.0006	0.0005	0.0001	1.112
H3-TW11GSC2-0-8S30	0.0002	0.0002	0.0000	1.086