Summing Nondetects When Computing Toxic Equivalents (TEQs)

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INTRODUCTION

The toxic equivalence (TEQ) methodology was developed to express the potential toxicity of a mixture as a single number, the assumption being that the toxicities of the individual chemical congeners are additive. However, as congener concentrations are often measured below their detection limits, the issue is raised of how to incorporate nondetects (NDs) in the computation of a total TEQ. The USEPA provides no guidance, other than substituting 0 and the detection limit, and reporting a range of possible TEQs (USEPA, 2008).

OBJECTIVE

The aim of this study is to examine two approaches for the computation of a total TEQ: substitution of one-half the method detection limit (MDL/2) for each nondetect, and the Kaplan-Meier (KM) method.

METHOD

Dioxin and furan concentrations measured in water (FIGURE 1), sediment (FIGURE 2), and sport fish (FIGURE 3) samples collected by the Regional Monitoring Program for Water Quality in the San Francisco Estuary (RMP) in 2009 were used to calculate, where possible, total TEQs for each sample.

FIGURE 1

FIGURE 2

FIGURE 3

SUBSTITUTION METHOD

The 17 individual dioxin and furan concentrations were multiplied by their respective toxicity equivalence factors (TEFs), as compiled by the WHO (2005), with nondetects substituted with one half the method detection limit (ND=MDL/2), and the products summed to obtain a total TEQ.

KAPLAN-MEIER METHOD

The KM procedure takes nondetects at their face value, so instead of substituting one half the method detection limit, nondetects are expressed as their method detection limit. TABLE 1 shows an example calculation for one sport fish samples. With the KM procedure, the method detection limit values for NDs are multiplied by the congener's TEF so that the congener TEQ for HpCDF, 1,2,3,4,7,8,9- in the right-hand column is expressed as <0.000496 rather than as a detected 0.000248 resulting from substitution of one-half the method detection limit. The KM procedure takes NDs at face value, therefore, the five nondetect TEQs are combined with the 11 detected values (OCDD, 1,2,3,4,6,7,8,9- value which historically contributes 11% (TABLE 2), was rejected due to blank contamination) to produce an estimated mean of 0.0128. If we transform the equation for calculating the mean ($\mu = (x_0 + x_1 + x_2 + ... + x_{n-1})/n$), then the sum is equal to the mean multiplied by n. Therefore, multiplying the estimate of the mean (0.0128) by the number of observations (n = 16), the KM sum obtained without substituting any values for nondetects is 0.2052.

TABLE 1

Congener	Measured Concentrations	MDL/2	Toxic Equivalence Factors (TEFs)	Toxicity Equivalence Concentrations (ND = MDL/2)	Toxicity Equivalence Concentrations (KM Method)
HpCDD, 1,2,3,4,6,7,8-	0.09	-	0.01	0.0009	0.0009
HpCDF, 1,2,3,4,6,7,8-	0.06	-	0.01	0.0006	0.0006
HpCDF, 1,2,3,4,7,8,9-	ND (< 0.0496)	0.0248	0.01	0.000248	< 0.000496
HxCDD, 1,2,3,4,7,8-	0.061	-	0.1	0.0061	0.0061
HxCDD, 1,2,3,6,7,8-	0.059	-	0.1	0.0059	0.0059
HxCDD, 1,2,3,7,8,9-	ND (< 0.0496)	0.0248	0.1	0.00248	< 0.000496
HxCDF, 1,2,3,4,7,8-	ND (< 0.0496)	0.0248	0.1	0.00248	< 0.000496
HxCDF, 1,2,3,6,7,8-	ND (< 0.0496)	0.0248	0.1	0.00248	< 0.000496
HxCDF, 1,2,3,7,8,9-	0.052	-	0.1	0.0052	0.0052
HxCDF, 2,3,4,6,7,8-	ND (< 0.0496)	0.0248	0.1	0.00248	< 0.000496
OCDD, 1,2,3,4,6,7,8,9-	R	-	0.0003	-	-
OCDF, 1,2,3,4,6,7,8,9-	0.136	-	0.0003	0.0000408	0.0000408
PeCDD, 1,2,3,7,8-	0.076	-	1	0.076	0.076
PeCDF, 1,2,3,7,8-	0.054	-	0.03	0.00162	0.00162
PeCDF, 2,3,4,7,8-	0.125	-	0.3	0.0375	0.0375
TCDD, 2,3,7,8-	0.058	-	1	0.058	0.058
TCDF, 2,3,7,8-	0.107	-	0.1	0.0107	0.0107
Total TEQ	-	-	-	0.2127	0.2052

TABLE 1. Example of toxicity equivalence concentration (TEQ) calculation using substitution of half the method detection limit (MDL/2) and the Kaplan-Meier (KM) method for one sport fish sample. ND indicates a nondetect, R indicates the value was rejected and not used in the calculation.

KAPLAN-MEIER METHOD LIMITATIONS

> The KM procedure can not be used to calculate a total TEQ when all ND's have only one MDL, in such cases, the KM estimate of the mean equals that of substituting the method detection value for the nondetects (Helsel, 2005); this is unlikely when concentrations are multiplied by different TEFs.

> The KM procedure can not be used when there is a high ND value, higher than all TEQs from detected concentrations, for one of the highest-toxicity congeners (PeCDD, 1,2,3,7,8- and TCDD, 2,3,7,8- with TEFs of 1), in this case, no calculation procedure will give a reliable estimate of the total TEQ (Helsel, 2010).

> If the KM procedure could not be used, then we substituted 0 and the method detection limit for nondetects to obtain a best- and worst-case estimate, with the knowledge that the true value of the worst-case total TEQ may be much lower.

TABLE 2

Congener	Toxic Equivalence Factors (TEFs)	Mean	stdev	n
HpCDD, 1,2,3,4,6,7,8-	0.01	1	2.0	37
HpCDF, 1,2,3,4,6,7,8-	0.01	6	8.7	37
HpCDF, 1,2,3,4,7,8,9-	0.01	2	3.1	37
HxCDD, 1,2,3,4,7,8-	0.1	0	1.5	37
HxCDD, 1,2,3,6,7,8-	0.1	2	2.6	37
HxCDD, 1,2,3,7,8,9-	0.1	0	0.5	37
HxCDF, 1,2,3,4,7,8-	0.1	14	23.3	37
HxCDF, 1,2,3,6,7,8-	0.1	3	5.0	37
HxCDF, 1,2,3,7,8,9-	0.1	0	0.2	37
HxCDF, 2,3,4,6,7,8-	0.1	0	0.5	37
OCDD, 1,2,3,4,6,7,8,9-	0.0003	11	16.1	37
OCDF, 1,2,3,4,6,7,8,9-	0.0003	3	6.0	37
PeCDD, 1,2,3,7,8-	1	4	5.1	37
PeCDF, 1,2,3,7,8-	0.03	3	2.7	37
PeCDF, 2,3,4,7,8-	0.3	13	10.1	37
TCDD, 2,3,7,8-	1	3	2.9	37
TCDF, 2,3,7,8-	0.1	33	20.0	37

TABLE 2. Toxic equivalence factors (TEFs) and percent contributions of dioxins/furans to the Sum of Dioxins and Furans in sport fish samples (1994-2009).

RESULTS

WATER

Total TEQs were not estimable using the KM procedure for 18 out of 21 (86%) water samples as PeCDD, 1,2,3,7,8- and TCDD, 2,3,7,8-, the two highest-toxicity congeners, were reported as NDs, with the proportion of NDs for these samples ranging from 6 to 76 percent (TABLE 3). The best- and worst-case TEQ estimates were not very helpful due to their wide ranges ($mean$ = 45.1 (ppt ww), sd = 26.7, $range$ = 5.4 - 111.1, n = 18), but in general the higher the proportion of NDs the wider the estimated TEQ range (Kendall's tau = 0.5353, z = 3.0485, p = 0.002, n = 18). Three (14%) of the water samples had no NDs.

SEDIMENT

Total TEQs were not estimable using the KM procedure for 45 out of 47 (96%) sediment samples (TABLE 4). One sample because both PeCDD, 1,2,3,7,8- and TCDD, 2,3,7,8-, the two highest-toxicity congeners, were reported as NDs; proportion of NDs for this sample was 53%. The other 44 samples had no NDs. We were able to use the KM procedure to estimate the total TEQ value for only two (4%) of the sediment samples (BG20 and BG30).

SPORT FISH

We were able to estimate total TEQs using the KM procedure for all 34 sport fish composites (TABLE 5), although one sample (TABLE 5; Composite 13, 71%) was just above the level of censoring considered suitable for the KM method (70%; Antweiler and Taylor, 2008). The KM procedure estimates ($mean$ = 0.7487, sd = 0.3734) were found to be significantly less (FIGURE 4; paired t-test, t = 9.76, df = 33, p < 0.0005, n = 34) than those calculated using the substitution of MDL/2 for the NDs ($mean$ = 0.7587, sd = 0.3694). However, this does not mean the difference is important as a small among-replicate variance can result in a significant t-test, even though the magnitude of the difference may be small.

OCDD, 1,2,3,4,6,7,8,9- results were not available due to blank contamination for 31 out of the 34 (91%) sport fish samples. As OCDD, 1,2,3,4,6,7,8,9- historically contributed 11% to the sum of dioxins and furans in sport fish samples (TABLE 2) we wanted to examine the impact of this rejection on the use of the KM procedure as a reliable estimator. Using the knowledge that the sum of dioxins and furans for the remaining 16 congeners represented 89% of the historic "sum" we calculated a value for the missing OCDD, 1,2,3,4,6,7,8,9- concentration. This value was then combined with the other 16 sample congeners and the "new" total TEQ estimate (KM N; TABLE 5) compared with the original value (KM TEQ; TABLE 5). OCDD, 1,2,3,4,6,7,8,9- concentrations were found to be responsible for over- or underestimations of less than 0.2 percent ($mean$ $percent$ $difference$ = 0.0495, sd = 0.0663, $range$ = -0.0277 - 0.1851, n = 34); OCDD, 1,2,3,4,6,7,8,9- being one of the lowest-toxicity congeners (TABLE 2; TEF = 0.0003).

TABLE 3

Site Code	Region	Matrix	Date	% ND	best-case ND=0 TEQ (ppt ww)	worst-case ND=MDL TEQ (ppt ww)	No NDs TEQ (ppt ww)	KM TEQ (ppt ww)	Comments
SPB027W	San Pablo Bay	Dissolved	9/1/09	76	0.87	40.82	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
SU030W	Suisun Bay	Dissolved	9/2/09	71	1.01	55.34	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
SPB027W	San Pablo Bay	Particulate	9/1/09	47	16.27	61.91	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
SU030W	Suisun Bay	Particulate	9/2/09	53	12.48	66.75	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
BA30	South Bay	Total	8/26/09	6	80.32	106.12	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
BC10	Central Bay	Total	8/31/09	29	37.62	63.33	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
BC20	Central Bay	Total	8/28/09	47	0.22	41.90	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
BG20	Rivers	Total	9/3/09	41	7.26	98.75	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
CB027W	Central Bay	Total	8/31/09	35	30.55	58.84	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
CB029W	Central Bay	Total	8/28/09	41	32.12	63.91	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
SB054W	South Bay	Total	8/26/09	18	53.03	73.30	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
SB055W	South Bay	Total	8/27/09	6	100.91	123.31	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
SB057W	South Bay	Total	8/27/09	29	32.36	60.06	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
SPB027W	San Pablo Bay	Total	9/1/09	59	9.28	95.23	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
SPB028W	San Pablo Bay	Total	9/1/09	29	16.66	57.07	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
SPB029W	San Pablo Bay	Total	9/1/09	41	31.41	46.78	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
SU030W	Suisun Bay	Total	9/2/09	65	7.19	118.27	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
SU031W	Suisun Bay	Total	9/2/09	12	65.50	97.83	--	--	High toxicity analyte PeCDD, 1,2,3,7,8- was ND
CB028W	Central Bay	Total	8/27/09	0	--	--	71.94	--	No NDs
LSB038W	Lower South Bay	Total	8/24/09	0	--	--	409.35	--	No NDs
LSB039W	Lower South Bay	Total	8/25/09	0	--	--	190.50	--	No NDs

TABLE 3. Proportion of nondetects (ND) and toxicity equivalence concentrations (TEQ) using substitution and Kaplan-Meier (KM) method for 2009 water samples.

TABLE 5

Composite	Site Code	Region	Station Name	Common Name	Prep Preservation	% ND	ND=MDL/2 TEQ (ppt ww)	KM TEQ (ppt ww)	KM N (ppt ww)	% Difference KM TEQ vs. KM N	Comments
1	203BRKLEY	Central Bay	Berkeley (4)	Shiner Surfperch	Skin off	41	0.8348	0.8261	0.8263	-0.0159	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
2	203CENTRL	Central Bay	Central Bay (6)	White Croaker	Skin off	65	0.2541	0.2379	0.2379	-0.0277	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
3	203CENTRL	Central Bay	Central Bay (6)	White Croaker	Skin on, Scales Off	41	0.7752	0.7635	0.7636	-0.0110	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
4	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	59	0.4069	0.3948	0.3944	0.0947	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
5	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	53	0.5382	0.5276	0.5270	0.1103	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
6	203OAKLND	Central Bay	Oakland (2)	Shiner Surfperch	Skin off	12	1.2584	1.2564	1.2564	0.0000	
7	203SANFRN	Central Bay	San Francisco Waterfront (3)	Shiner Surfperch	Skin off	0	0.8982	0.8982	0.8982	0.0000	
8	204STHBAY	South Bay	South Bay (1)	White Croaker	Skin off	29	0.2127	0.2052	0.2048	0.1851	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
9	204STHBAY	South Bay	South Bay (1)	White Croaker	Skin on, Scales Off	59	0.4267	0.4129	0.4122	0.1751	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
10	204STHBAY	South Bay	South Bay (1)	Shiner Surfperch	Skin on, Scales Off	41	0.8500	0.8450	0.8446	0.0551	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
11	206SNPBLO	San Pablo Bay	San Pablo Bay (5)	Shiner Surfperch	Skin off	53	0.4814	0.4701	0.4697	0.0963	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
12	203BRKLEY	Central Bay	Berkeley (4)	Shiner Surfperch	Skin off	35	0.8039	0.7959	0.7959	0.0077	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
13	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	71	0.2522	0.2221	0.2218	0.1324	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
14	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	53	0.5495	0.5351	0.5351	-0.0050	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
15	203OAKLND	Central Bay	Oakland (2)	Shiner Surfperch	Skin off	18	1.5928	1.5906	1.5906	0.0000	
16	203SANFRN	Central Bay	San Francisco Waterfront (3)	Shiner Surfperch	Skin off	24	0.7574	0.7535	0.7531	0.0533	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
17	204STHBAY	South Bay	South Bay (1)	White Croaker	Skin off	53	0.6839	0.6676	0.6674	0.0250	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
18	204STHBAY	South Bay	South Bay (1)	White Croaker	Skin on, Scales Off	18	1.6466	1.6446	1.6449	-0.0149	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
19	204STHBAY	South Bay	South Bay (1)	Shiner Surfperch	Skin on, Scales Off	29	0.8837	0.8798	0.8795	0.0354	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
20	206SNPBLO	San Pablo Bay	San Pablo Bay (5)	Shiner Surfperch	Skin off	53	0.6017	0.5926	0.5919	0.1222	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
21	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	53	0.5469	0.5373	0.5365	0.1469	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
22	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	12	1.0098	1.0076	1.0077	-0.0129	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
23	204STHBAY	South Bay	South Bay (1)	White Croaker	Skin off	59	0.3371	0.3236	0.3231	0.1753	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
24	204STHBAY	South Bay	South Bay (1)	White Croaker	Skin on, Scales Off	29	1.5055	1.5007	1.5011	-0.0234	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
25	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	53	0.7246	0.7071	0.7064	0.0991	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
26	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	29	1.1771	1.1714	1.1714	0.0023	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
27	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	47	0.5237	0.5117	0.5114	0.0747	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
28	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	53	0.9870	0.9780	0.9772	0.0824	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
29	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	59	0.3460	0.3300	0.3299	0.0361	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
30	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	47	0.7666	0.7551	0.7551	-0.0084	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
31	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	47	0.5902	0.5805	0.5798	0.1190	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
32	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	53	1.0750	1.0617	1.0619	-0.0207	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
33	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin off	53	0.5906	0.5777	0.5776	0.0096	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.
34	203OAKLND	Central Bay	Oakland (2)	White Croaker	Skin on, Scales Off	53	0.9072	0.8936	0.8938	-0.0140	Analyte OCDD, 1,2,3,4,6,7,8,9- was rejected value.

TABLE 5. Proportion of nondetects (ND) and toxicity equivalence concentrations (TEQ) using substitution and Kaplan-Meier (KM) method for 2009 sport fish samples.

FIGURE 4

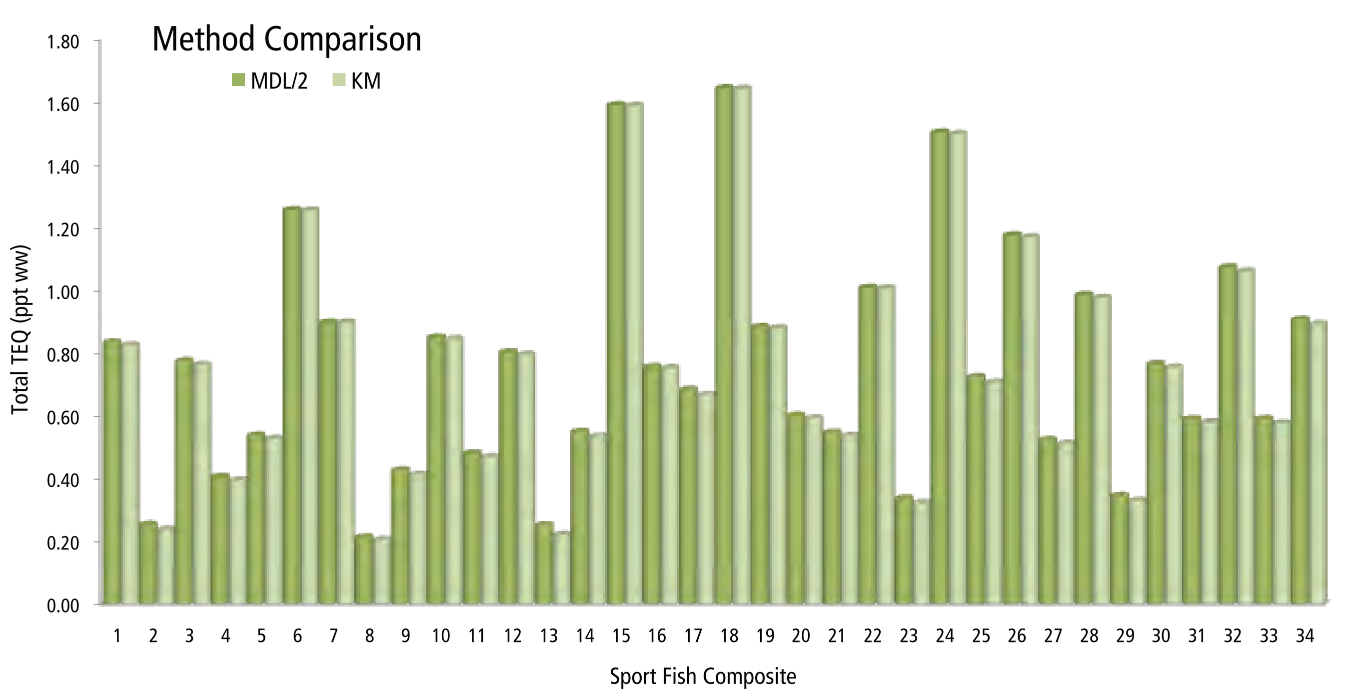

TABLE 4

Site Code	Region	Matrix	Date	% ND	best-case ND=0 TEQ (ppt dw)	worst-case ND=MDL TEQ (ppt dw)	ND=MDL/2 TEQ (ppt dw)	No NDs TEQ (ppt dw)	KM TEQ (ppt dw)	Comments
BG20	Rivers	sediment	9/23/09	12	--	--	0.1505	--	0.1496	
BG30	Rivers	sediment	9/23/09	24	--	--	0.3848	--	0.3823	
SU042S	Suisun Bay	sediment	9/22/09	53	0.0259	0.0889	--	--	--	High toxicity analytes PeCDD, 1,2,3,7,8- & TCDD, 2,3,7,8- were ND
BF21	Suisun Bay	sediment	9/22/09	0	--	--	--	2.0649	--	No NDs
SU001S	Suisun Bay	sediment	9/22/09	0	--	--	--	0.3329	--	No NDs
SU015S	Suisun Bay	sediment	9/22/09	0	--	--	--	3.7734	--	No NDs
SU016S	Suisun Bay	sediment	9/22/09	0	--	--	--	2.3783	--	No NDs
SU073S	Suisun Bay	sediment	9/22/09	0	--	--	--	1.9715	--	No NDs
SU085S	Suisun Bay	sediment	9/23/09	0	--	--	--	0.4993	--	No NDs
SU090S	Suisun Bay	sediment	9/23/09	0	--	--	--	0.5490	--	No NDs
SU117S	Suisun Bay	sediment	9/22/09	0	--	--	--	0.8238	--	No NDs
BD31	San Pablo Bay	sediment	9/18/09	0	--	--	--	1.7091	--	No NDs
SPB001S	San Pablo Bay	sediment	9/21/09	0	--	--	--	2.0020	--	No NDs
SPB002S	San Pablo Bay	sediment	9/18/09	0	--	--	--	1.2572	--	No NDs
SPB015S	San Pablo Bay	sediment	9/21/09	0	--	--	--	2.3389	--	No NDs
SPB016S	San Pablo Bay	sediment	9/21/09	0	--	--	--	1.7660	--	No NDs
SPB071S	San Pablo Bay	sediment	9/21/09	0	--	--	--	1.9614	--	No NDs
SPB080S	San Pablo Bay	sediment	9/21/09	0	--	--	--	2.0558	--	No NDs
SPB135S	San Pablo Bay	sediment	9/18/09	0	--	--	--	1.6692	--	No NDs
SPB136S	San Pablo Bay	sediment	9/21/09	0	--	--	--	1.5953	--	No NDs
BC11	Central Bay	sediment	9/17/09	0	--	--	--	2.6847	--	No NDs
CB001S	Central Bay	sediment	9/18/09	0	--	--	--	2.4404	--	No NDs
CB002S	Central Bay	sediment	9/16/09	0	--	--	--	2.6296	--	No NDs
CB016S	Central Bay	sediment	9/16/09	0	--	--	--	2.2320	--	No NDs
CB043S	Central Bay	sediment	9/18/09	0	--	--	--	2.5820	--	No NDs
CB044S	Central Bay	sediment	9/17/09	0	--	--	--	1.0081	--	No NDs
CB058S	Central Bay	sediment	9/16/09	0	--	--	--	1.7570	--	No NDs
CB075S	Central Bay	sediment	9/18/09	0	--	--	--	2.0211	--	No NDs
CB121S	Central Bay	sediment	9/18/09	0	--	--	--	1.5217	--	No NDs
BA41	South Bay	sediment	9/16/09	0	--	--	--	2.7830	--	No NDs
SB002S	South Bay	sediment	9/16/09	0	--	--	--	2.6533	--	No NDs
SB015S	South Bay	sediment	9/17/09	0	--	--	--	2.6141	--	No NDs
SB016S	South Bay	sediment	9/17/09	0	--	--	--	2.2506	--	No NDs
SB060S	South Bay	sediment	9/16/09	0	--	--	--	2.0053	--	No NDs
SB061S	South Bay	sediment	9/16/09	0	--	--	--	1.5825	--	No NDs
SB069S	South Bay	sediment	9/17/09	0	--	--	--	2.2814	--	No NDs
SB073S	South Bay	sediment	9/17/09	0	--	--	--	2.2538	--	No NDs
SB106S	South Bay	sediment	9/16/09	0	--	--	--	2.8809	--	No NDs
BA10	Lower South Bay	sediment	9/15/09	0	--	--	--	3.9236	--	No NDs
LSB001S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.0881	--	No NDs
LSB002S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.8811	--	No NDs
LSB015S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.1680	--	No NDs
LSB016S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.5260	--	No NDs
LSB071S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.6062	--	No NDs
LSB082S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.0585	--	No NDs
LSB097S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.4096	--	No NDs
LSB108S	Lower South Bay	sediment	9/15/09	0	--	--	--	3.1695	--	No NDs

TABLE 4. Proportion of nondetects (ND) and toxicity equivalence concentrations (TEQ) using substitution and Kaplan-Meier (KM) method for 2009 sediment samples.

DISCUSSION

Substitution of one-half the detection limit for each nondetect is the most common method used by environmental scientists today for dealing with censored data. However, substitution can produce an invasive pattern alien to the concentrations actually in the samples, resulting in generally poor estimates and incorrect statistical tests (Helsel, 2005; Helsel, 2009). Best- and worst-case estimates, especially when reported as wide ranges, may be the poorest approach of all as it often leads to the common but simplistic method of substitution of one-half the detection limit in order to obtain a single TEQ value (Helsel, 2010).

This does not have to be the case. In most situations there are better methods for handling censored data, such as the Kaplan-Meier (KM) procedure, an alternative method widely used in the fields of medical and industrial statistics (Helsel, 2005). The KM method is a nonparametric maximum likelihood procedure that provides better, more statistically defensible estimates of descriptive statistics than substitution (Antweiler and Taylor, 2008).

CONCLUSION

This small study, using real world environmental data, illustrates some of the pitfalls and limitations associated with incorporating nondetects into the calculation of total TEQs. These difficulties, however, should not be taken as a reason to employ simplistic substitution methods that can provide biased and unreliable estimates. Instead, environmental researchers need to expand their horizons as alternative methods to substitution are available for estimating descriptive statistics, performing hypothesis tests, and computing correlation coefficients and regression equations. The use of such methods can only provide better, more accurate scientific interpretations (Helsel, 2006).

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