

### Toxic Equivalents Guidance for Dioxin and Dioxin-like Compound Case Study 1

ATSDR received a petition from a state agency to evaluate environmental data from a site named Clam Bay used for growing commercial shellfish. Historical and current industrial activities surrounding the bay have resulted in contamination of the underlying sediment with dioxin and dioxin-like compounds. ATSDR accepted the petition and evaluated dioxin data from surface sediment grab samples collected at various locations throughout the bay. The laboratory results for 17 dioxin or dioxin-like compounds are shown in Table 1 for one of these samples.

Table 1  
Results for a single sediment sample<sup>1</sup>

Compound	Result (ng/kg dw)
1,2,3,4,6,7,8-HpCDD	16
1,2,3,4,6,7,8-HpCDF	3.5
1,2,3,4,7,8,9-HpCDF	0.27
1,2,3,4,7,8-HxCDD	<0.17
1,2,3,4,7,8-HxCDF	0.44
1,2,3,6,7,8-HxCDD	0.59
1,2,3,6,7,8-HxCDF	0.30
1,2,3,7,8,9-HxCDD	0.34
1,2,3,7,8,9-HxCDF	<0.10
1,2,3,7,8-PeCDD	<0.15
1,2,3,7,8-PeCDF	0.37
2,3,4,6,7,8-HxCDF	0.35
2,3,4,7,8-PeCDF	0.30
2,3,7,8-TCDD	0.04
2,3,7,8-TCDF	0.44
OCDD	151
OCDF	7.6

Review the data provided above and answer the following question.

- 1) What TEQ value should the health assessor use for the sample data shown in Table 1 in their health evaluation?

---

<sup>1</sup> NOTE: Sample data are provided for a hypothetical site. For the purposes of this case study, assume these data are of a known and high quality, and meet the data quality objectives for the health evaluation.

## Supplemental Case Study Examples – Questions and Answers

Answer:

### Step 1: Perform a data quality review.

In this example, it is assumed that the data are of a known and high quality and meet all data quality objectives for the health evaluation in question. There are no R-qualified (i.e., rejected) results and therefore no data must be removed before calculating the TEQ.

The example data set is for a single sample without replicate or duplicate analysis, and no further data processing of duplicates is required.

This example includes concentrations for 17 congeners, three of which are reported as non-detect. As described in Section 3.4 of the guidance document, the KM method can be used to calculate TEQs for data sets with non-detect results, if there are least three detected concentrations. The data for this environmental sample meets this criterion and the KMcalc Excel macro will apply the KM method.

### Step 2: Calculate the TEQ<sup>2</sup>

#### *Enter Site Information in the KMCalc Macro*

Enter the date, site name, sample media, and any additional notes in the blue-shaded cells found in rows 4 through 7 of the "OPTION 1- Calculations" spreadsheet. Then enter the units for all congeners in cell B9. Note that all congener concentrations must be entered in the same units.

	A	B
1	<b>TEQ Calculation for a Single Sample</b>	
2		
3	<b>INPUT DATA</b>	
4	Date:	1-Jan
5	Site Name:	Clam Bay
6	Media:	Sediment
7	Notes:	Sample 1
8		
9	Units for all congener concentrations →	ng/kg

#### *Insert the data in the KMcalc Excel file*

Enter congener-specific analytical data into the blue-shaded cells starting in Row 13. Begin by entering or selecting congener shorthand names from the drop-down lists in the first column.

---

<sup>2</sup> To demonstrate the process for calculating TEQs, this case study outlines the approach using ATSDR's Excel spreadsheet that already has the KMcalc macro loaded. Health assessors can alternatively load the KMcalc to an existing Excel workbook that contains the dioxin and dioxin-like compounds analytical results. Refer to Section 3.5 and Appendix B of the guidance for more detail.

## Supplemental Case Study Examples – Questions and Answers

Once the shorthand congener names are entered, the following three columns will automatically populate with each congener's category, CAS number, and full name. Users should then enter congener concentrations and data qualifiers in columns E and F, respectively. Refer to Appendix B.1 of the guidance for specific instructions and examples for entering these data. Note that data qualifiers may only be entered as one of four options: U, J, UJ, or a blank cell. Any other inputs in the qualifier column will result in a pop-up error message.

Shorthand congener names, concentrations, and qualifiers in the blue highlighted cells.							Clear All Data
Shorthand Congener Name (Enter or select from drop-down list)	Category	CAS Number	Full Congener Name	Concentration (Enter all concentrations in the same units)	Qualifier (U, J, or UJ) (Enter or select from the drop-down list)	TEF	
1,2,3,4,6,7,8-HpCDD	Dioxin	35822-46-9	1,2,3,4,6,7,8-Heptachloro dibenzo-p-dioxin	16		0.01	
1,2,3,4,6,7,8-HpCDF	Furan	67562-39-4	1,2,3,4,6,7,8-Heptachloro dibenzofuran	3.5		0.01	
1,2,3,4,7,8,9-HpCDF	Furan	55673-89-7	1,2,3,4,7,8,9-Heptachloro dibenzofuran	0.27		0.01	
1,2,3,4,7,8-HxCDD	Dioxin	39227-28-6	1,2,3,4,7,8-Hexachloro dibenzo-p-dioxin	0.17	U	0.1	
1,2,3,4,7,8-HxCDF	Furan	70648-26-9	1,2,3,4,7,8-Hexachloro dibenzofuran	0.44		0.1	
1,2,3,6,7,8-HxCDD	Dioxin	57653-85-7	1,2,3,6,7,8-Hexachloro dibenzo-p-dioxin	0.59		0.1	
1,2,3,6,7,8-HxCDF	Furan	57117-44-9	1,2,3,6,7,8-Hexachloro dibenzofuran	0.3		0.1	
1,2,3,7,8,9-HxCDD	Dioxin	19408-74-3	1,2,3,7,8,9-Hexachloro dibenzo-p-dioxin	0.34		0.1	
1,2,3,7,8,9-HxCDF	Furan	72918-21-9	1,2,3,7,8,9-Hexachloro dibenzofuran	0.1	U	0.1	
1,2,3,7,8-PeCDD	Dioxin	40321-76-4	1,2,3,7,8-Pentachloro dibenzo-p-dioxin	0.15	U	1	
1,2,3,7,8-PeCDF	Furan	57117-41-6	1,2,3,7,8-Pentachloro dibenzofuran	0.37		0.03	
2,3,4,6,7,8-HxCDF	Furan	60851-34-5	2,3,4,6,7,8-Hexachloro dibenzofuran	0.35		0.1	
2,3,4,7,8-PeCDF	Furan	57117-31-4	2,3,4,7,8-Pentachloro dibenzofuran	0.3		0.3	
2,3,7,8-TCDD	Dioxin	1746-01-6	2,3,7,8-Tetrachloro dibenzo-p-dioxin	0.04		1	
2,3,7,8-TCDF	Furan	51207-31-9	2,3,7,8-Tetrachloro dibenzofuran	0.44		0.1	
OCDD	Dioxin	3268-87-9	1,2,3,4,6,7,8,9-Octachloro dibenzo-p-dioxin	151		0.0003	
OCDF	Furan	39001-02-0	1,2,3,4,6,7,8,9-Octachloro dibenzofuran	7.6		0.0003	

### Run the Macro and Obtain Results

After all data have been entered, click the "Run TEQ Calculations". The orange shaded cells in Rows 4 through 6 will then present the results: the TEQ concentration and units, as well as the qualifier to apply to the calculated TEQ concentration.

OUTPUT DATA	
Use this TEQ concentration:	0.67148
TEQ concentration units:	ng/kg
Use this qualifier:	No qualifier
Sensitivity analysis result:	Passed Sensitivity Test
<input type="button" value="Run TEQ Calculations"/>	

In this example, the calculated TEQ is equal to 0.671 ng/kg and does not require a qualifier.

### Step 3: Sensitivity Analyses and Quality Control checks

This example does not include any non-detect observations or rejected results. As such, sensitivity analyses are not required and the calculated TEQ is appropriate for use in the health evaluation. Health assessors are encouraged to document their calculations and have an experienced colleague replicate their results.

**Toxic Equivalents Guidance for Dioxin and Dioxin-like Compound  
Case Study 2**

ATSDR received a petition from a private citizen and an environmental organization to conduct a public health assessment of dioxin and dioxin-like contamination in wild game living in a flood plain area downstream of a chemical manufacturing plant. Deer samples were collected from the area of concern as well as from a reference area upstream of the plant. Table 2 presents the laboratory results for 17 dioxin or dioxin-like compounds measured in one sample of deer liver.

Table 2  
Results for a single deer liver sample<sup>3</sup>

Compound	Result (pg/g fat)	Qualifier
1,2,3,4,6,7,8-HpCDD	1,720	
1,2,3,4,6,7,8-HpCDF	376	
1,2,3,4,7,8,9-HpCDF	29.0	
1,2,3,4,7,8-HxCDD	18.2	
1,2,3,4,7,8-HxCDF	47.3	R
1,2,3,6,7,8-HxCDD	63.4	
1,2,3,6,7,8-HxCDF	32.2	
1,2,3,7,8,9-HxCDD	36.5	
1,2,3,7,8,9-HxCDF	5.0	U
1,2,3,7,8-PeCDD	16.1	
1,2,3,7,8-PeCDF	39.7	
2,3,4,6,7,8-HxCDF	37.6	
2,3,4,7,8-PeCDF	32.2	
2,3,7,8-TCDD	1.0	U
2,3,7,8-TCDF	47.3	
OCDD	162,32	
OCDF	817	

Review the data provided above and answer the following question.

- 1) What TEQ value should the health assessor use for the sample data shown in Table 1 in their health evaluation?

---

<sup>3</sup> NOTE: Sample data are provided for a hypothetical site. For the purposes of this case study, assume these data are of a known and high quality, and meet the data quality objectives for the health evaluation.

## Supplemental Case Study Examples – Questions and Answers

Answer:

### Step 1: Perform a data quality review

In this example, it is assumed that the data are of a known and high quality and meet all data quality objectives for the health evaluation in question. There is one R-qualified (i.e., rejected) result that needs to be removed before calculating the TEQ.

The example data set is for a single sample without replicate or duplicate analysis, and no further data processing of duplicates is required.

This example includes concentrations for 17 congeners, one of which was rejected, and two of which are reported as non-detect. As described in Section 3.4 of the guidance document, the KM method can be used to calculate TEQs for data sets with non-detect results, if there are least three detected concentrations. The data for this environmental sample meets this criterion and the KMcalc Excel macro will apply the KM method.

### Step 2: Calculate the TEQ<sup>4</sup>

#### Enter Site Information in the KMCalc Macro

Enter the date, site name, sample media, and any additional notes in the blue-shaded cells found in rows 4 through 7 of the "OPTION 1- Calculations" spreadsheet. Then enter the units for all congeners in cell B9. Note that all congener concentrations must be entered in the same units.

	A	B
1	<b>TEQ Calculation for a Single Sample</b>	
2		
3	<b>INPUT DATA</b>	
4	Date: January, 1	
5	Site Name: Site Name	
6	Media: Deer Liver	
7	Notes: Sample 1	
8		
9	Units for all congener concentrations →	pg/g fat

<sup>4</sup> To demonstrate the process for calculating TEQs, this case study outlines the approach using ATSDR's Excel spreadsheet that already has the KMcalc macro loaded. Health assessors can alternatively load the KMcalc macro to an existing Excel workbook that contains the dioxin and dioxin-like compounds analytical results. Refer to Section 3.5 and Appendix B of the guidance for more detail.

## Supplemental Case Study Examples – Questions and Answers

Insert the data in the KMcalc Excel file

Enter congener-specific analytical data into the blue-shaded cells starting in Row 13. Begin by entering or selecting congener shorthand names from the drop-down lists in the first column.

Once the shorthand congener names are entered, the following three columns will automatically populate with each congener's category, CAS number, and full name. Users should then enter congener concentrations and data qualifiers in columns E and F, respectively. Refer to Appendix B.1 of the guidance for specific instructions and examples for entering these data. Note that data qualifiers may only be entered as one of four options: U, J, UJ, or a blank cell. Any other inputs in the qualifier column will result in a pop-up error message.

							Clear All Data
Shorthand congener names, concentrations, and qualifiers in the blue highlighted cells.							
Shorthand Congener Name (Enter or select from drop-down list)	Category	CAS Number	Full Congener Name	Concentration (Enter all concentrations in the same units)	Qualifier (U, J, or UJ) (Enter or select from the drop-down list)	TEF	
1,2,3,4,6,7,8-HpCDD	Dioxin	35822-46-9	1,2,3,4,6,7,8-Heptachloro dibenzo-p-dioxin	1,720		0.01	
1,2,3,4,6,7,8-HpCDF	Furan	67562-39-4	1,2,3,4,6,7,8-Heptachloro dibenzofuran	376		0.01	
1,2,3,4,7,8,9-HpCDF	Furan	55673-89-7	1,2,3,4,7,8,9-Heptachloro dibenzofuran	29		0.01	
1,2,3,4,7,8-HxCDD	Dioxin	39227-28-6	1,2,3,4,7,8-Hexachloro dibenzo-p-dioxin	18.2		0.1	
1,2,3,6,7,8-HxCDD	Dioxin	57653-85-7	1,2,3,6,7,8-Hexachloro dibenzo-p-dioxin	63.4		0.1	
1,2,3,6,7,8-HxCDF	Furan	57117-44-9	1,2,3,6,7,8-Hexachloro dibenzofuran	32.2		0.1	
1,2,3,7,8,9-HxCDD	Dioxin	19408-74-3	1,2,3,7,8,9-Hexachloro dibenzo-p-dioxin	36.5		0.1	
1,2,3,7,8,9-HxCDF	Furan	72918-21-9	1,2,3,7,8,9-Hexachloro dibenzofuran	5	U	0.1	
1,2,3,7,8-PeCDD	Dioxin	40321-76-4	1,2,3,7,8-Pentachloro dibenzo-p-dioxin	16.1		1	
1,2,3,7,8-PeCDF	Furan	57117-41-6	1,2,3,7,8-Pentachloro dibenzofuran	39.7		0.03	
2,3,4,6,7,8-HxCDF	Furan	60851-34-5	2,3,4,6,7,8-Hexachloro dibenzofuran	37.6		0.1	
2,3,4,7,8-PeCDF	Furan	57117-31-4	2,3,4,7,8-Pentachloro dibenzofuran	32.2		0.3	
2,3,7,8-TCDD	Dioxin	1746-01-6	2,3,7,8-Tetrachloro dibenzo-p-dioxin	1	U	1	
2,3,7,8-TCDF	Furan	51207-31-9	2,3,7,8-Tetrachloro dibenzofuran	47.3		0.1	
OCDD	Dioxin	3268-87-9	1,2,3,4,6,7,8,9-Octachloro dibenzo-p-dioxin	162,32		0.0003	
OCDF	Furan	39001-02-0	1,2,3,4,6,7,8,9-Octachloro dibenzofuran	817		0.0003	

Run the Macro and Obtain Results

After all data have been entered, click the "Run TEQ Calculations". The orange shaded cells in Rows 4 through 6 will then present the results: the TEQ concentration and units, as well as the qualifier to apply to the calculated TEQ concentration.

OUTPUT DATA	
Use this TEQ concentration:	77.3708
TEQ concentration units:	pg/g fat
Use this qualifier:	No qualifier
Sensitivity analysis result:	Passed Sensitivity Test
<input type="button" value="Run TEQ Calculations"/>	

In this example, the calculated TEQ is equal to 77.37 pg/g fat and does not require a qualifier.

### Step 3: Sensitivity Analyses and Quality Control Checks

ATSDR's Excel spreadsheet with the KMcalc macro already loaded provides results for the sensitivity analyses for handling non-detects. In this example, the sample data passed this test. This means that the relative percent difference (RPD) between the upper and lower bound TEQs

*Supplemental Case Study Examples – Questions and Answers*

estimating while substituting non-detects with zero and full detection limits, respectively, was below 50 percent. Refer to Section 3.6 and Appendix C of the guidance for more detail.

An additional sensitivity analysis should be performed for rejected data. Since we excluded the R-qualified result for 1,2,3,4,7,8-HxCDF from the TEQ calculations, the initial TEQ estimate should be compared to a TEQ that includes the R-qualified result.

<b>Approach to Handling R-Qualified Results</b>	<b>Estimated TEQ (pg/g)</b>
Initial TEQ based on the KM method excluding R-qualified result	77.37
TEQ based on the KM method including R-qualified result	82.01

Calculate the RPD between the initial TEQ and the TEQ when including R-qualified data.

$$RPD = \left( \frac{|Value_1 - Value_2|}{(Value_1 + Value_2) \div 2} \right) \times 100$$

$$RPD = \left( \frac{|77.37 - 82.01|}{(77.37 + 82.01) \div 2} \right) \times 100$$

$$RPD = 5.8 \text{ percent}$$

The RPD between the initial TEQ and the TEQ including the R-qualified result is 5.8 percent, indicating that the exclusion of rejected data has minimal impact on the overall TEQ. In this case, health assessors would proceed with the initial TEQ.

The TEQ calculation passed both sensitivity analyses and the calculated value of 77.37 pg/g fat is therefore appropriate to use in the health evaluation. Health assessors are encouraged to document their calculations and have an experienced colleague replicate their results.