ATSDR Toxic Equivalents Procedure for Dioxin and Dioxin-like Compounds Evaluation

Citation:

[ATSDR] Agency for Toxic Substances and Disease Registry. 2025. Toxic Equivalents Procedure for Dioxin and Dioxin-like Compounds. Atlanta, GA: U.S. Department of Health and Human, Services, Public Health Service. September 3.

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List of Abbreviations

ADS Associate Director for Science
AhR aryl hydrocarbon receptor

ATSDR Agency for Toxic Substances and Disease Registry
CASRN Chemical Abstracts Service Reference Number

CV comparison value
DLC dioxin-like compound
EDG Exposure Dose Procedure

EMPC estimated maximum possible concentration

EPC exposure point concentration

ISM incremental sampling methodology

KM Kaplan-Meier MRL Minimal Risk Level

OCDAPS Office of Capacity Development and Applied Prevention Science

OCHHA Office of Community Health Hazard Assessment

PAH polycyclic aromatic hydrocarbon

PCB polychlorinated biphenyl

PCDD polychlorinated dibenzo-p-dioxin PCDF polychlorinated dibenzofuran PHA public health assessment

RfD reference dose

RPD relative percent difference

2,3,7,8-TCDD 2,3,7,8-tetrachlorodibenzo-p-dioxin TEC toxic equivalent concentration

TEF toxic equivalent factor

TEQ toxic equivalent

USEPA U.S. Environmental Protection Agency

95UCL 95 percent upper confidence limit of the arithmetic mean

WHO World Health Organization

Note

This evaluation procedure mentions software applications by name (e.g., Microsoft Excel). Use of these trade names is for identification purposes only and does not constitute an endorsement of their use.

1. Introduction

When multiple chemicals in the same chemical class have sufficiently similar toxicological properties, toxic equivalents (TEQs) can be used to express the numerous chemicals' overall toxicity as a single value. This document presents the Agency for Toxic Substances and Disease Registry's (ATSDR's) procedure for calculating TEQs for dioxin and dioxin-like compounds (DLCs)—a class of related halogenated aromatic hydrocarbons that are specially handled in ATSDR public health evaluations.

Focus of This Procedure

This procedure walks health assessors through the process of calculating the TEQ for *a single sample* of dioxin and dioxin-like compounds.

Once TEQs have been calculated for all samples in an exposure unit following the steps in this procedure, health assessors should then apply principles in other procedure documents (e.g., ATSDR, 2019a; 2020a) to determine what TEQ to use as the exposure point concentration for the health evaluations.

This procedure presents ATSDR's recommended statistical procedures for calculating TEQs and specifically considers uncertainties associated with environmental sampling data that contain non-detects. Calculating TEQs with non-detect results is not a new concept, and many textbooks, articles, and other publications present different approaches for doing so. However, health assessors are expected to follow the computational approaches presented in this procedure, which address specific nuances of environmental data for dioxin and DLCs. Computational approaches other than those prescribed in this procedure should not be used, unless first approved by an Associate Director for Science (ADS) group.

This procedure supersedes previous versions of ATSDR procedure on dioxins and DLCs. The current procedure, in addition to incorporating advanced statistical approaches to handling non-detect results, includes the most recent World Health Organization (WHO) toxic equivalent factor (TEF) values from 2022 [WHO 2024].

1.1. When to Use This Procedure

During the public health assessment process, health assessors perform many activities, such as: developing a conceptual site model, evaluating exposure pathways, identifying exposure units, compiling and reviewing environmental data, and screening those data against health-based comparison values (CVs). ATSDR has developed other procedure to assist health assessors with these and many other steps in public health evaluations. Health assessors should follow the procedure in this document when working on sites with measured concentrations of dioxins and DLCs in any environmental media (e.g., soil, groundwater, surface water, fish tissue, outdoor air, and indoor air).

This procedure specifically outlines how to transform data for an environmental sample analyzed for dioxin and DLCs into a single TEQ and should be applied prior to screening data against CVs and calculating exposure point concentrations (EPCs) for health evaluations. The procedure was not developed to address how to use and interpret the results for those evaluations. But briefly, health assessors should treat TEQs like concentrations of any other environmental contaminant. In this case, health assessors should evaluate TEQs using comparison values, health guidelines, and other resources

specific to 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD). Health assessors should also be mindful that several individually measured chemicals accounted for in the TEQ have their own CVs and/or health guidelines and should therefore be evaluated separately—meaning, these chemicals should both (1) be evaluated individually and (2) factored into the TEQ calculations. These chemicals currently include:

- 2,3,7,8-Tetrachloro dibenzo-p-dioxin (CASRN: 1746-01-6)
- 1,2,3,6,7,8-Hexachloro dibenzo-p-dioxin (CASRN: 57653-85-7)
- 1,2,3,7,8,9-Hexachloro dibenzo-p-dioxin (CASRN: 19408-74-3)
- 2,3,4,7,8-Pentachloro dibenzofuran (CASRN: 57117-31-4)

Using Calculated TEQs

Health assessors can use the TEQs calculated following the procedures outlined in this procedure to evaluate both cancer and non-cancer effects. Evaluate the calculated TEQs like any other contaminant in the public health assessment process, by first screening the TEQ against the recommended cancer and non-cancer CV. If the calculated TEQ meets or exceeds a CV, health assessors should determine the EPC for that exposure unit and then estimate non-cancer hazards and cancer risks.

Once health assessors have calculated a TEQ for each environmental sample with the methods described in this document, they should screen both the calculated TEQs and the measured concentrations of the four chemicals listed above against ATSDR recommended CVs for **both cancer and non-cancer** (e.g., environmental media evaluation guides [EMEGs] and cancer risk evaluation guides [CREGs]). If any of the individual sample TEQs or chemical measurements exceed applicable CVs in a potential or completed exposure pathway, health assessors must perform a more detailed risk evaluation.

For these evaluations, health assessors estimate EPCs using the calculated TEQs for all environmental samples collected within an exposure unit. To do so, they should follow applicable ATSDR Exposure Dose Procedure (EDG) on how to define an exposure unit (ATSDR, 2020b) and on how to calculate EPCs (e.g., ATSDR, 2019a; 2020a). Health assessors should use these EPCs to calculate doses and then compare those doses to appropriate health guidelines (e.g., minimal risk levels [MRLs], reference doses [RfDs], cancer slope factors [CSFs]), like any other contaminant in the public health assessment process. For dioxin and DLCs, this means applying health guidelines for 2,3,7,8-TCDD to calculated TEQs, as well as applying available health guidelines for the four chemicals specified above.

1.2. Topics Not Covered by This Procedure

This procedure specifically addresses approaches for evaluating environmental sampling data for dioxin and DLCs. This document is just one part of a larger series of ATSDR procedure documents that outline approaches for evaluating exposures to environmental contamination. Moreover, the procedure applies to the calculation of TEQs for dioxin and DLCs based on environmental sampling data collected with discrete, composite, and incremental methods. This procedure does not apply to:

TEQ calculations for Polycyclic Aromatic Hydrocarbons (PAHs). ATSDR has developed separate
procedure (ATSDR, 2022) that applies specifically to PAHs and explains the toxicity weighting
scheme health assessors should apply for this separate class of chemicals.

Calculating EPCs from multiple environmental samples. ATSDR has developed separate procedure (e.g., ATSDR, 2019a; 2020a) that describes the process of calculating EPCs with discrete sampling data and non-discrete sampling data. After using this procedure to determine TEQs for individual samples in an exposure unit, health assessors should then apply the other procedure documents to determine EPCs on a TEQ basis for the entire exposure unit.

While health assessors can use this procedure to calculate TEQs for dioxin and DLC data collected via any sampling strategy, they must use sampling specific procedure when calculating EPCs.

1.3. Resources for Further Information

This procedure was developed to make TEQ calculations for dioxin and DLCs a straightforward process. For additional background information on the general EPA approach followed in this procedure, health assessors are referred to the following sources:

- United States Environmental Protection Agency's (EPA's) User Guide Uniform Federal Policy
 Quality Assurance Project Plan Template for Soils Assessment of Dioxin Sites (EPA, 2011).
- WHO's Recommended Toxicity Equivalence Factors (TEFs) for Human Health Risk Assessments of 2,3,7,8-Tetrachlorodibenzo-p-dioxin and DLCs (DeVito et al. 2024).

Some health assessors may want to access additional resources for information on the advanced topics mentioned in this document. In those cases, health assessors should:

- Review Dr. Dennis Helsel's paper on estimating TEQs for dioxin and DLCs. (Helsel 2010)
- Consult with their ADS group for other resources. ATSDR recommends this option to ensure that
 all health assessors consistently rely on a common approach when calculating TEQs, rather than
 having health assessors individually seeking input from different (and perhaps inappropriate or
 conflicting) sources.

1.4. How to Use This Procedure

Health assessors will find all TEQ procedure in this document's text. Appendix A includes a glossary of key terms, Appendix B describes special considerations for samples with non-detects, and Appendix C provides example TEQ calculations. Additional information is provided in text boxes, as follows:

Key Point

Blue text boxes concisely summarize major elements of this TEQ procedure.

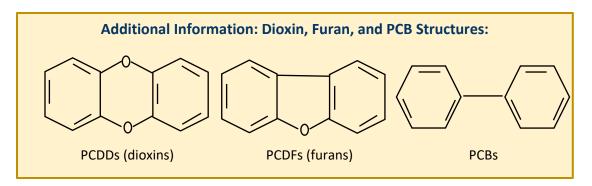
Additional Information

Yellow text boxes provide scientific background information on issues related to TEQ calculations.

2. Background

The term "dioxin and DLCs" refers to a wide range of compounds in three chemical classes: polychlorinated dibenzo-p-dioxins (PCDD), polychlorinated dibenzofurans (PCDF), and polychlorinated biphenyls (PCBs). These three chemical classes represent structurally and toxicologically similar halogenated aromatic compounds (EPA, 2011). The individual compounds within each class are referred to throughout the remainder of this document as "congeners."

Congeners within these three chemical classes (e.g., PCDDs, PCDFs, and PCBs) have similar structures, but varying physical and chemical properties based on the position of chlorine atoms. PCDD and PCDF congeners have two benzene rings joined by a single or double oxygen bridge, while PCBs consist of two benzene rings joined by a carbon-to-carbon bond. Varying numbers of chlorines are attached to the carbons of the congeners, and congener names are assigned based on the position and number of those chlorine atoms. See the yellow box below for the basic structure of PCDDs, PCDFs, and PCBs.



While PCDDs, PCDFs, and PCBs comprise almost 420 individual congeners, only a small subset of these congeners are considered to have dioxin-like toxicity and are therefore included in TEQ calculations. Congeners with dioxin-like toxicity are those known to bind to the aryl hydrocarbon receptor (AhR) in humans and to elicit toxic or biochemical responses. Table 1 (found at the end of this procedure) lists these congeners—any PCDD, PCDF, or PCB congeners not listed in Table 1 should not be factored into TEQ calculations.

Key Point: PCDDs, PCDFs, and PCBs with dioxin-like toxicity

Dioxin and DLC Groups	Total Number of Congeners	Number of Congeners with Known Dioxin-like Toxicity	
PCDDs -	75	7	
Dioxins			
PCDFs -	135	10	
Furans			
PCBs	209	12	

The term "dioxin and DLCs" refers to the seven PCDDs, ten PCDFs, and 12 PCBs with dioxin-like toxicity. Only these congeners are included in TEQ calculations.

2.1. What are TEQs and When to Use Them

TEQs provide a means for transforming measurements of numerous different congeners analyzed from one environmental sample to a single value that can be used for health assessment purposes. They are calculated to represent the overall toxicity of complex mixtures of PCDD, PCDF, and PCB congeners, relative to a single benchmark compound. In the case of dioxin and DLCs, the toxicity of each individual congener is weighted against that of 2,3,7,8-tetrachlorodibenzo-p-dioxin (2,3,7,8-TCDD), historically considered the most toxic member of these chemical classes. Most dioxins and DLCs are thought to have much lower toxicity than TCDD, except for 1,2,3,7,8-pentachlorodibenzo-p-dioxin, which is considered approximately 40% as toxic as 2,3,7,8-TCDD. Measured concentrations and detection limits of each congener and the congeners' corresponding weighting factors are used to characterize the toxicity of dioxin and DLCs.

To calculate TEQs, toxic equivalent factors (TEFs) have been assigned to each dioxin and DLC congener. TEFs are assigned by comparing the relative toxicity of individual congeners to that of 2,3,7,8-TCDD, based on detailed scientific review of chemical structures and toxicological databases. Currently, values range from 0.00003 to 0.4. A TEF of 0.1 indicates that the congener is 1/10th as toxic as 2,3,7,8-TCDD.

TEF consensus values developed by the WHO and accepted by ATSDR are shown in Table 1, at the end of this procedure (DeVito et al., 2024). These values replace 2005 WHO TEF values used previously (Van den Berg et al., 2006). The TEFs are for mammalian species and should be used for all TEQ calculations by health assessors to support public health evaluations. The specific TEF values used represent toxicity relative to 2,3,7,8-TCDD (EPA, 2009; DeVito et al. 2024). WHO periodically reviews and updates these values, and ADS groups will inform health assessors of any notable future updates. Note that EPA recommends that TEFs be used for all effects mediated through aryl hydrocarbon receptor binding by dioxin and DLCs, including cancer and noncancer effects (EPA, 2009).

To calculate the TEQ for an environmental sample, the concentrations of individual congeners are first multiplied by their respective TEFs to produce congener-specific toxic equivalent concentrations (TEC). The individual TECs are then summed to obtain a total TEQ for the sample. The two equations used to calculate TEQs are shown in the blue box below.

Key Point: How to calculate a TEQ

Equation 1:

Equation 2:

$$TEC_i = C_i \times TEF_i \qquad TEQ = \sum_{i=1}^{k} (TEC_i)$$

Where:

- TEC_i is the toxic equivalent concentration of the ith individual congener in the sample.
- C_i is the measured concentration of the ith individual congener in the sample.
- *TEF*_i is the individual toxic equivalent factor.
- TEQ is the toxic equivalent for the environmental sample.
- k is the number of congeners that make up the TEQ.

While calculating TEQs provides a useful technique to transform measured concentrations of numerous congeners into a single value, health assessors should be familiar with the following underlying

assumptions that went into developing TEFs, before applying them to public health evaluations (Safe, 1990).

- 1. The compounds exert toxicity through a common receptor-mediated mechanism.
- 2. The effects of the individual congeners within the mixtures are additive.
- 3. The individual congeners have similarly shaped dose-response curves.

Overall, the TEQ framework provides a scientifically justified, health protective, and widely accepted method for evaluating toxicity of mixtures of dioxin and DLCs. However, the method has inherent uncertainties and may not capture the true health risks of all exposure scenarios (NAS, 2006).

3. Procedure Recommendation: Calculating TEQs for a Single Sample

This section presents ATSDR's recommended approach to calculating TEQs for evaluating health implications of exposures to dioxin and DLCs. Since health assessors will frequently encounter data sets that include non-detect results, this section includes information on how to handle "censored data"— a term commonly used to describe data sets including non-detect observations. Health assessors should review this section and the additional information in Appendix B and C before applying this procedure.

Key Point: General strategy for calculating TEQs with non-detect results

To calculate TEQs for an environmental sample, health assessors should:

- Review and prepare the data for TEQ calculations (Section 3.3).
- Calculate the TEQ using ATSDR's EPC Tool (Section 3.5).
- Complete sensitivity analyses to evaluate the influence of different methods to handle non-detects and rejected results (Section 3.6).

3.1. General Approach for Calculating TEQs

The general approach to calculate TEQs differs for environmental samples without non-detect observations (see Section 3.1.1) and with non-detect observations (Section 3.1.2). However, the same software applications (Section 3.2), data processing steps (Section 3.3), use of ATSDR's Exposure Point Concentration tool (Section 3.4), sensitivity analyses (Section 3.6), and quality control checks (Section 3.7) apply to both scenarios. The remainder of this section describes the general approach for data sets without and with non-detects.

3.1.1. Environmental Samples without Non-detect Observations

To illustrate the general TEQ computational approach shown in Section 2.1 and applicable to environmental samples <u>without</u> non-detect observations, this section presents a hypothetical soil sample in which seven DLCs were measured, and all had detected concentrations. Refer to the text box later in this section for the specific values. To calculate the TEQ for this sample, the detected results for the seven dioxin congeners are first multiplied by applicable TEFs to calculate TECs, and then summed to calculate the TEQ for the sample.

In this example, the TEQ for the soil sample is 3.45 ng-TEQ/kg. The health assessor would first compare this TEQ concentration to the CV for 2,3,7,8-TCDD. If the TEQ concentration exceeds

the CV, the TEQ would then be used in the health effects evaluation, following guidelines for 2,3,7,8-TCDD.

Note that the TEQ calculated in this example is presented in units of ng-TEQ/kg soil. This is consistent with ATSDR's preferred approach for reporting the TEQ concentrations, as explained in the blue box below. Health assessors should report all calculated TEQs following this naming convention.

Additional Information: Example TEQ Calculations from a Data set without non-detect results from a Single Soil Sample

Dioxin Congener	Analytical Result (ng/kg)	TEF ^a (unitless)	TEC ^b (ng/kg)
2,3,7,8-TCDD	1.7	1	1.7
1,2,3,7,8-PeCDD	0.18	0.4	0.072
1,2,3,4,7,8-HxCDD	0.26	0.09	0.0234
1,2,3,6,7,8-HxCDD	2.1	0.07	0.147
1,2,3,4,6,7,8-HpCDD	25	0.05	1.25
1,2,3,7,8,9-HxCDD	0.77	0.05	0.0385
OCDD	220	0.001	0.22
2,3,7,8-TCDD TEQ $^{\circ}$ = 3.45 ng-TEQ/k			5 ng-TEQ/kg

^a2022 WHO TEFs as presented in Table 1 at the end of this procedure.

With this simple illustration, health assessors should recognize that TEQs are weighted sums of the individual congeners, with weights based on each congeners' relative toxicity to 2,3,7,8-TCDD. Another way to consider the result from the example above is that exposure to the measured concentrations of the seven different DLC congeners is essentially equivalent to exposure to 3.45 ng/kg of 2,3,7,8-TCDD.

Key Point: Reporting Calculated TEQs

Chemical concentrations are typically reported in units of mass of the chemical per mass or volume of the sampled media (e.g., air, soil, sediment, groundwater, etc.). Health assessors should report all calculated TEQs in units of measurement that include "TEQ" in the unit's numerator. This is particularly important so that TEQ results are not confused with congener-specific results. Several examples of this TEQ naming convention are shown below.

- Soil and sediment: pg-TEQ/kg and ng-TEQ/kg
- Indoor and outdoor air: pg-TEQ/m³ and ng-TEQ/m³
- Groundwater and surface water: pg-TEQ/L and ng-TEQ/L

^bTEC for each congener determined by Equation 1.

^c2,3,7,8-TCDD TEQ for sample determined by Equation 2.

This hypothetical example is only shown to illustrate the TEQ computational approach. In most cases, health assessors will encounter samples in which some dioxin and DLC congeners are detected and others are not. The following section reviews general approaches for those scenarios.

3.1.2. Environmental Samples with Non-detect Observations

Non-detects are valid measurements in which the concentration of the contaminant of interest is too low to measure with confidence. Sampling reports typically present non-detect results as being less than a specified limit (e.g., "<25 ng/kg"), with that limit being either a method detection limit or a quantification limit. In these cases, health assessors can only conclude that the actual contaminant level is somewhere between zero and the specified level. Nonetheless, non-detects still provide useful information and should be included in TEQs.

ATSDR's preferred approach to calculate a TEQ from an environmental sample with non-detect observations follows Dr. Dennis Helsel's approach of Kaplan-Meier (KM) estimation (Helsel, 2012). This non-parametric approach uses an unbiased framework for handling non-detect observations in TEQ calculations. The KM estimation is built into the EPC Tool. Specific considerations for environmental samples with non-detect results are summarized in Appendix B.

3.2. Software Applications

Health assessors should use the EPC Tool developed by ATSDR to calculate TEQs for environmental samples with dioxin and DLC data. A link to the EPC Tool can be found in the resources section of ATSDR's Public Health Assessment Site Tool (PHAST) or accessed here https://cdcposit.cdc.gov/epctool/. The EPC Tool will calculate TEQs for samples without non-detects following the process described in Section 3.1. For samples with non-detect results, the tool will process data qualifiers per ATSDR procedures and will provide summary statistics (i.e., maximum concentration and 95UCL) for TEQs using the KM method. Details regarding how the TEQs are calculated for non-detects are presented in Appendix B, instructions on how to use the EPC Tool are provided in Section 3.4, and the process is demonstrated with an example data set in Appendix C.

Health assessors may notice that EPA provides publicly available Microsoft Excel spreadsheet tools that calculate TEQs for dioxin and DLCs with the KM method. These tools, however, were designed to accommodate incremental sampling data (e.g., with inputs for triplicate sampling results) and therefore do not apply to all sampling scenarios; and other aspects of the TEQ calculations do not align with ATSDR's procedure (e.g., how to process environmental samples when the highest result is a non-detect). Health assessors are therefore encouraged to use ATSDR's EPC Tool for determining EPCs.

3.3. Data Processing Steps

Regardless of whether a given sample includes non-detect results, health assessors should always complete the following two data processing steps:

 Perform a data quality review. Before proceeding with TEQ calculations, health assessors should review their environmental sampling data to confirm the data are of high quality and meet the data quality objectives for the health evaluation in question. Any R-qualified (e.g., rejected) results should be removed from the data set. TEQs should never be calculated with R-qualified data.

Health assessors should, however, take note of any R-qualified values that are removed from a data set to conduct subsequent sensitivity analyses. These analyses should be completed to ensure that the decision to exclude R-qualified data does not substantially impact the final TEQ. Sensitivity analyses are described in Section 3.6 and should be completed whenever R-qualified results are removed.

Identify and process duplicate samples and replicate analyses. Two commonly used approaches to characterize measurement precision in the analysis of environmental samples are through analyzing duplicate samples (i.e., two samples collected from the exact same place and time) or conducting replicate analyses of a single environmental sample (i.e., two separate laboratory analyses of the same sample). Health assessors should not use both measurements from duplicate samples or replicate analyses in health evaluations, because doing so artificially assigns greater weight to these samples or analyses. Instead, health assessors should reduce results from duplicate samples or replicate analyses into the result for a single sampling event.

For dioxin and DLCs, the preferred approach is to calculate average congener concentrations from duplicate samples or replicate analyses, and then use those averages to represent the single sampling event to calculate the TEQ for CV comparisons and health evaluations. As an example, assume a laboratory received a single soil sample and analyzed that sample in replicate (i.e., the laboratory generated two different profiles of congener concentrations for the same sample). To determine the TEQ for this sample, health assessors should first average the congener concentrations from each replicate following the steps outlined in this procedure; and then enter the single average concentration for each congener from the two replicates to determine the TEQ of the overall sampling event using the EPC Tool. This procedure should be applied for both duplicate samples and replicate analyses.

3.4. Calculating TEQs and EPCs with ATSDR's EPC Tool

Health assessors should utilize the EPC Tool found here https://cdcposit.cdc.gov/epctool/, to determine what concentrations should be entered into PHAST. Users will need to download and fill out the Data Import Template Excel file and will need to ensure the appropriate CAS Registry Number (CASRN) is entered in for each of the DLCs. It is suggested that health assessors copy and paste the CASRNs from Table 1 below. The remaining inputs (e.g., exposure unit, concentration, etc.) will also need to be added accurately to properly calculate the EPC for each exposure unit. For data below the limit of detection, the value reported for the limit of detection should be entered, not a zero. A zero is not permitted and will cause errors with the EPC Tool. For more information on using the EPC Tool, see ATSDR's Exposure Point Concentration (EPC) Tool User Guide (ATSDR 2024).

For each congener and exposure unit in the Data Import Template Excel file, the EPC Tool will calculate an EPC based on the number of congener sample records associated with the exposure unit. In addition, the EPC Tool will calculate a TEQ EPC for the exposure unit based on the exposure unit's individual sample TEQs. The EPC Tool uses the same algorithm to generate TEQ EPCs as it does for individual congener EPCs. For more information on the EPC Tool's algorithm for generating EPCs, see ATSDR's Exposure Point Concentration Procedure for Discrete Sampling (ATSDR 2019a).

Additional Information: Viewing Individual Sample TEQs

The EPC Tool returns EPCs on an exposure-unit basis and does not report TEQs for individual samples. In most analyses, individual sample TEQs will not be needed, and health assessors should use the EPC Tool results as they are reported. If, however, users wish to see the individual sample TEQs generated internally within the EPC Tool, these can be displayed by assigning a separate exposure unit to each sample with dioxin or DLC results in the Data Import Template Excel file. Because the EPC Tool calculates EPCs on an exposure-unit basis, the EPC Tool will associate each sample with a different exposure unit and will calculate and report the individual sample TEQs as the exposure unit TEQ EPCs.

3.5. Calculating TEQs with ATSDR's EPC Tool

As described in Section 3.1, health assessors should use ATSDR's EPC Tool to calculate TEQs for environmental samples with and without non-detect results. This single tool applies Equations 1 and 2 (as shown in Section 2.1) for samples without non-detects and the Kaplan Meier (KM) method for samples with non-detects. In one rare exception (i.e., for samples with fewer than three detected results), the EPC Tool cannot be used to calculate TEQs and health assessors are referred to Appendix B.

Health assessors must confirm their Excel spreadsheets include the following necessary data inputs. Refer to the example shown in Appendix C for instructions on how these inputs must be formatted for use with the EPC Tool. The following list describes important considerations for each input:

- Exposure Unit
 - Health Assessors can enter more than a single exposure unit into the EPC Tool at a single time by specifying different Exposure Units in column A.
- Contaminant Name and CASRN
 - Health Assessors are encouraged to copy and paste this information from Table 1
 (at the end of this procedure document) and omit any congeners in Table 1 that were not tested for.
- Media
 - Health Assessors need to select the most appropriate media from the dropdown list in the input file.
- Concentrations:
 - All inputs for congener concentrations must be numeric values. Symbols, letters (e.g., "<" or lab qualifiers in the concentration field), and extraneous blank spaces

- will result in formula errors. Non-detect results should be replaced with their respective LODs as zero is not permitted.
- All congener concentrations must be in the same units (e.g., ng/kg or ng/m³), which is usually the case for environmental sampling data; meaning, laboratories typically will not use two different units of measurement when reporting concentrations for congeners within a single environmental sample. However, if data are from multiple laboratories, the units must match, and conversions may be necessary. These units, however, should not be entered with congener concentrations in the spreadsheet macro; the EPC Tool will return an error when units are typed into the concentration field. There is a separate column for the units. The calculated TEQ will be in the same units as the individual congener concentrations.
- Congener data do not need to be sorted.

Detected Flag:

A "U" qualifier must be entered as a 0 in the "DetectedFlag" column for all non-detect observations. This is because the computational algorithm recognizes the "0" as a non-detect observation. In cases where a laboratory uses other letters or conventions to represent non-detects (e.g., some laboratories might report them as "ND" or "<MDL"), health assessors must also mark the column entry a "0". Positive detections, including estimated concentrations with a "J" flag, must be entered with a "1" in the "DetectedFlag" column.</p>

Sample ID:

 The Sample ID should be entered for each contaminant listed. Errors will result if two identical contaminants (i.e., same CASRN are entered as having the same Sample ID.

Once data are properly entered into Excel, health assessors can use the EPC Tool in just the same way as any other contaminant. When DLCs from Table 1 are present, the tool will automatically calculate TEQs. However, before using those TEQs, health assessors should first check the results of the sensitivity analyses described in Section 3.6.

3.6. Sensitivity Analyses

Health assessors should complete two sensitivity analyses to ensure that the initial TEQ estimate is not heavily influenced by the KM method used to handle non-detects or by exclusion of R-qualified results. The EPC Tool automatically performs the calculations for the sensitivity analysis on non-detects, but health assessors must rerun the EPC Tool to complete the sensitivity analysis on R-qualified results, as described below.

- Sensitivity Analyses for Handling Non-Detects. Health assessors should use the EPC Tool's built in methods for all dioxin and DLC TEQ calculations for data sets containing non-detect results.
 However, to confirm that the calculated TEQs are not heavily influenced by the KM method, the
 - EPC Tool will compare the TEQs calculated with the KM method to lower- and upper-bound TEQ estimates with the following two substitution methods:
 - Lower-bound TEQ estimate: All non-detect congeners are set to detections with a concentration of zero by the EPC Tool.
 - Upper-bound TEQ estimate: All non-detect congeners are set to detections with a concentration of their detection limits by the EPC Tool.

The EPC Tool will automatically calculate the lowerand upper-bound TEQ estimates—users do not need to perform these calculations manually. After reviewing the lower and upper bound TEQ

Additional Information: Sensitivity Analysis

The sensitivity analyses described in Section 3.6 are used to determine whether the TEQ calculated according to the procedure is acceptable to use for health assessment purposes. The health assessor should not use the sensitivity analysis TEQs for their health evaluations. The appropriate TEQs to use in health evaluations are calculated by the EPC Tool following the procedures in Section 3.1.

estimates, users should always use the TEQ estimates that are based on the detection limit as the concentration for non-detect records.

Once the values are calculated, the EPC Tool will compare the upper-bound TEQ to the lower-bound TEQ by calculating the relative percent difference (RPD) between the two values. An RPD of greater than 50 percent suggests the method for replacing non-detects has an unacceptably large influence on the results. If this occurs for any sample used to calculate a TEQ EPC, the EPC Tool will flag the results and health assessors should consult with their ADS group on how to proceed. If the TEQ EPC is not flagged, health assessors should proceed with CV comparisons and health effects evaluations using the initial EPC Tool results. The equation to calculate the RPD between two values is shown in Equation 3.

Equation 3:

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

Health assessors who are working in ATSDR's EPC Tool will be provided with a data flagged result if this sensitivity test is failed for any sample used to calculate a TEQ EPC. The "Notes" field of the TEQ EPC will identify the names of the samples that failed the sensitivity test. Additional information about the TEQ EPC is supplied when "Download All Statistics" is selected.

Sensitivity Analyses for Handling R-qualified Data (e.g., rejected). As described in Section 3.3, R-qualified data should never be included in initial TEQ estimates. However, to confirm that exclusion of R-qualified results does not have an unacceptably large influence on the calculated TEQs, health assessors should use the EPC Tool to recompute the TEQs by including the rejected results. The EPC Tool does not perform this calculation automatically, so health assessors will need to run the tool twice—once with and once without the R-qualified results—to complete the analysis. This computation can only be performed if a concentration was included with the

R-qualified results. To calculate TEQs for individual samples, follow the steps in the text box in Section 3.4.

After generating individual sample TEQs including R-qualified results, health assessors should calculate the RPD between these values and the TEQ estimates without R-qualified results. If the RPDs are less than 50 percent for all samples, health assessors should proceed with CV comparisons and health effects evaluations using the initially calculated EPC Tool results that do not include the R qualified results. If the RPD exceeds 50 percent for any sample and if the TEQ including the R-qualified value is at a level of health concern, health assessors should still use the initial EPC Tool results in the health evaluation but acknowledge the limitations associated with excluding the rejected values. The health assessor should also consider whether additional sampling is needed to reduce the uncertainties associated with the rejected values. Influence of rejected results will be greatest when congeners with relative high toxicity (e.g., a TEQ close to 1.0) are R-qualified.

3.7. Quality Control Checks

Health assessors are encouraged to have a colleague double-check their calculations. It is always good practice to have colleagues review calculations that support PHA conclusions, especially TEQ calculations used in health effects evaluations. To facilitate this review, health assessors should document their calculations and ask an experienced colleague to replicate the results.

3.8. Special Considerations

While ATSDR developed this procedure to apply to a broad range of site-specific scenarios, some environmental data sets will present unique challenges for calculating TEQs. In general, health assessors should consult with their ADS group when they encounter any site-specific scenarios or other circumstances not sufficiently covered by the general practice presented earlier in this procedure. Health assessors should also discuss with their ADS group how to handle estimated maximum probable concentration (EMPC) data when calculating TEQs. These data are briefly described below.

Some dioxin results may contain EMPC values (e.g., when a congener peak is present at an acceptable signal-to-noise ratio, but ion abundance criteria are not met for definitive identification of that congener) (EPA, 2011). These data are generally further qualified with a "J" flag for values that are estimated and a "U" flag for non-detect values. In general, "J" flagged EMPC values may be treated as estimated values and U-qualified results may be considered non-detected values, and used in TEQ calculations following the process prescribed in Sections 3.3 to 3.4. However, given that EMPC values may overestimate the TEQ, a sensitivity analysis should be performed to assess the influence of EMPC results on calculated TEQs (EPA 2011). Health assessors should perform a sensitivity analysis by calculating TEQs while excluding all EMPC values. When estimated TEQs are considerably different with and without these data, health assessors should contact their ADS group on how to proceed.

4. References

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Table 1. WHO 2022 Mammalian TEFs for Dioxin and DLCs

	Congener		Shorthand	
CASRN	Class	Full Congener Name	Congener Name ^a	TEF ^b
1746-01-6	Dioxin	2,3,7,8-Tetrachloro dibenzo-p-dioxin	2,3,7,8-TCDD	1
40321-76-4	Dioxin	1,2,3,7,8-Pentachloro dibenzo-p-dioxin	1,2,3,7,8-PeCDD	0.4
39227-28-6	Dioxin	1,2,3,4,7,8-Hexachloro dibenzo-p-dioxin	1,2,3,4,7,8-HxCDD	0.09
57653-85-7	Dioxin	1,2,3,6,7,8-Hexachloro dibenzo-p-dioxin	1,2,3,6,7,8-HxCDD	0.07
19408-74-3	Dioxin	1,2,3,7,8,9-Hexachloro dibenzo-p-dioxin	1,2,3,7,8,9-HxCDD	0.05
35822-46-9	Dioxin	1,2,3,4,6,7,8-Heptachloro dibenzo-p-dioxin	1,2,3,4,6,7,8-HpCDD	0.05
3268-87-9	Dioxin	1,2,3,4,6,7,8,9-Octachloro dibenzo-p-dioxin	OCDD	0.001
51207-31-9	Furan	2,3,7,8-Tetrachloro dibenzofuran	2,3,7,8-TCDF	0.07
57117-41-6	Furan	1,2,3,7,8-Pentachloro dibenzofuran	1,2,3,7,8-PeCDF	0.01
57117-31-4	Furan	2,3,4,7,8-Pentachloro dibenzofuran	2,3,4,7,8-PeCDF	0.1
70648-26-9	Furan	1,2,3,4,7,8-Hexachloro dibenzofuran	1,2,3,4,7,8-HxCDF	0.3
57117-44-9	Furan	1,2,3,6,7,8-Hexachloro dibenzofuran	1,2,3,6,7,8-HxCDF	0.09
72918-21-9	Furan	1,2,3,7,8,9-Hexachloro dibenzofuran	1,2,3,7,8,9-HxCDF	0.2
60851-34-5	Furan	2,3,4,6,7,8-Hexachloro dibenzofuran	2,3,4,6,7,8-HxCDF	0.1
67562-39-4	Furan	1,2,3,4,6,7,8-Heptachloro dibenzofuran	1,2,3,4,6,7,8-HpCDF	0.02
55673-89-7	Furan	1,2,3,4,7,8,9-Heptachloro dibenzofuran	1,2,3,4,7,8,9-HpCDF	0.1
39001-02-0	Furan	1,2,3,4,6,7,8,9-Octachloro dibenzofuran	OCDF	0.002
32598-13-3	PCB	3,3',4,4'-Tetrachlorobiphenyl	3,3',4,4'-tetraCB (PCB	0.0003
70362-50-4	PCB	3,4,4',5-Tetrachlorobiphenyl	3,4,4',5-tetraCB (PCB	0.006
32598-14-4	PCB	2,3,3',4,4'-Pentachlorobiphenyl	2,3,3',4,4'-pentaCB	0.00003
74472-37-0	PCB	2,3,4,4',5-Pentachlorobiphenyl	2,3,4,4',5-pentaCB	0.00003
31508-00-6	PCB	2,3',4,4',5-Pentachlorobiphenyl	2,3',4,4',5-pentaCB	0.00003
65510-44-3	PCB	2,3',4,4',5'-Pentachlorobiphenyl	2',3,4,4'5-pentaCB	0.00003
57465-28-8	PCB	3,3',4,4',5-Pentachlorobiphenyl	3,3'4,4',5-pentaCB	0.05
38380-08-4	PCB	2,3,3',4,4',5-Hexachlorobiphenyl	2,3,3',4,4',5-hexaCB	0.00003
69782-90-7	PCB	2,3,3',4,4',5'-Hexachlorobiphenyl	2,3,3',4,4',5'-hexaCB	0.00003
52663-72-6	PCB	2,3',4,4',5,5'-Hexachlorobiphenyl	2,3',4,4',5,5'-hexaCB	0.00003
32774-16-6	PCB	3,3',4,4',5,5'-Hexachlorobiphenyl	3,3',4,4',5,5'-hexaCB	0.005
39635-31-9	РСВ	2,3,3',4,4',5,5'-Heptachlorobiphenyl	2,3,3',4,4',5,5'- heptaCB (PCB 189)	0.00003

^aPCBs are named by the number and position of the chlorine atoms around the biphenyl ring. They are also sometimes referred to by their specific congener number, as shown in parentheses. For example, 3,3',4,4'-tetrachlorobiphenyl may be referred to by the shorthand name of 3,3',4,4'-TCB or PCB-77.

^bSource: Mammalian TEFs as published in DeVito M, Bokkers B, van Duursen M, van ede K, Feeley M, et al. 2024. The 2022 World Health Organization reevaluation of human and mammalian toxic equivalency factors for polychlorinated dioxins, dibenzofurans and biphenyls. Regulatory Toxicology and Pharmacology 146 (2024) 105525.

Appendices

Appendix A. Glossary

Censored Data: A term commonly used to describe data sets including non-detect observations.

Detection Limit. For environmental sampling, detection limits (often referred to as method detection limits) are thresholds below which measured concentrations are not significantly different from a blank signal, at a specified level of probability. Measurements above detection limits are evidence of a nonzero signal at a given probability, confirming that the analyte of interest is present in the sample.

Environmental Sample. A collected quantity of air, water, soil, food, or other media in which contamination levels are measured, whether directly in the field or at a laboratory.

Estimated maximum probable concentration (EMPC). Some dioxin results may contain EMPC values. This designation is used when a congener peak is present during laboratory analysis at an acceptable signal-to-noise ratio, but ion abundance criteria are not met for definitive identification of that congener (EPA, 2011). These data should still be used in the public health assessment process, and they are generally further qualified with a "J" flag for values that are estimated and a "U" flag for non-detect values.

Exposure Point Concentration (EPC). The representative contaminant concentration within an exposure unit or area in an exposure pathway to which persons are exposed for acute, intermediate, or chronic durations during the past, present, or future.

Dioxin-like. DLCs are structurally related groups of chemicals from the family of halogenated aromatic hydrocarbons. In this group, we include chlorinated dibenzo-p-dioxins, chlorinated dibenzofurans, and certain PCBs that have dioxin-like structural characteristics ("non-ortho-" and "mono-ortho-" substitutions).

Kaplan-Meier (KM). Kaplan-Meier is a non-parametric standard method for calculating statistics for data sets included censored data. In the context of this procedure, Kaplan-Meier method should be applied when calculating TEQs for an environmental sample that has non-detect observations.

Non-parametric methods. Non-parametric methods are statistical methods that do not assume data have a known shape or distribution. These methods can be applied with little information about the underlying distribution, including instances where details of the data distribution are not known. In this procedure, health assessors use non-parametric Kaplan-Meier methodto estimate toxicity equivalents for data sets with non-detect results.

Toxic Equivalent Concentration (TEC). The TEC is calculated as a congener's concentration multiplied by its TEF. The TEC is calculated as an intermediate step of the TEQ estimation.

Toxic Equivalent Factor (TEF). The TEF is based on the relative potency of the compound to the benchmark compound. A TEF of 0.1 indicates that the compound is $1/10^{th}$ as toxic as the benchmark compound, while 1 indicates that it is as toxic as the benchmark compound.

Toxic Equivalents (TEQ). Calculated values that represent the overall toxicity of a complex mixture of congeners, relative to a single benchmark compound (e.g., the most toxic compound in that family).

Appendix B: Special Considerations for Environmental Samples with Non-Detects

ATSDR's preferred approach to calculating TEQs for dioxin and DLCs for a single sample that includes non-detect results is to use the KM method, which is built into the EPC Tool. However, this method does not perform well for data sets with very few detected results (Helsel, 2010) and therefore is only used in the EPC Tool to calculate TEQs for environmental samples with at least three detected congeners. For example, if a laboratory analyzed an environmental sample for 17 DLC congeners, the EPC Tool would apply the KM method only if at least three of those congeners have detected concentrations.

This appendix describes the computational approaches used in the EPC Tool for environmental samples with fewer than three detected congeners and for environmental samples with three or more detected congeners. It also describes how the EPC Tool determines whether to consider calculated TEQs as detects or non-detects.

Calculating TEQs for Environmental Samples with Fewer than Three Detected Congeners

For an environmental sample with fewer than three detected congeners, the KM method should not be used. In this case, the total TEQ in the sample is uncertain. The TEQ's lower bound is the sum of the detected congener concentrations multiplied by their respective TEFs, and the TEQ's upper bound equals the TEQ's lower bound plus the detection limits of the non-detect congeners multiplied by their respective TEFs. The actual TEQ falls somewhere within the range of the TEQ upper and lower bounds. For samples with fewer than three detected congeners, the EPC Tool uses the TEQ's upper bound as the sample's TEQ.

$$TEQ_{lower} = \sum C_{id} \times TEF_{id}$$

Where C_{id} is the concentration of the ith detected congener and TEF_{id} is the toxic equivalent factor of the ith congener.

Health assessors should also examine whether the one or two detected congeners were measured at concentrations of potential health concern. If the detections were for any of the congeners listed in Section 1.1, health assessors should compare the measured concentrations of these congeners to their corresponding CVs.

Calculating TEQs for Environmental Samples with Three or More Detected Congeners

For environmental samples with at least three detected congeners and at least one non-detect congener, the EPC calculates TEQs using the KM method. In cases where the lowest or highest TEC is a non-detect, special considerations apply for the KM method calculations. The EPC Tool will account for these considerations, described here:

An environmental sample with the lowest TEC reported as a non-detect: If the lowest TEC across all congeners is a non-detect, the non-detect observation will be replaced in the KM method calculation with a detected concentration equal to the value of the detection limit. If more than one congener has the lowest TEC, the EPC Tool changes the non-detect observation to a detection for only one of them. If

multiple records with the lowest TEC are a mixture of detects and non-detects, the EPC Tool does not change any records.

An environmental sample with the highest TEC reported as a non-detect: In the unlikely event that the highest TEC across all congeners is a non-detect, the EPC Tool will consider this value as a detected concentration at its detection limit in the KM method calculation. If more than one congener has the highest TEC, the EPC Tool changes the non-detect observation to a detection for only one of them. If multiple records with the highest TEC are mixture of detects and non-detects, the EPC Tool does not change any records.

Determining Whether TEQs Are Considered as Detects or Non-detects

For a sample with both detected and non-detect congeners, the sample's TEQ could be considered as either a detect or a non-detect depending on the extent to which the non-detect congeners contribute to the overall TEQ. The EPC Tool decides whether sample TEQs will be considered as detects or as non-detects using the following algorithm:

- 1. Multiply the detected congener concentrations by their TEFs and sum the results to get a detected congener TEQ for the sample.
- 2. Multiply the non-detect congener detection limits by their TEFs and sum the results to get a non-detect congener TEQ for the sample.
- 3. Divide the non-detect congener TEQ by the sum of the detected and non-detect congener TEQs.
- 4. If the result of step 3 is more than 0.8, the EPC Tool treats the sample TEQ as a non-detect. Otherwise, the EPC Tool considers the sample TEQ to be a detection.

These calculations are based on the original detect/non-detect classification for each congener in the sample and do not reflect any changes made as a result of the procedures in this appendix.

Appendix C. Example TEQ Calculations Using the ATSDR EPC Tool

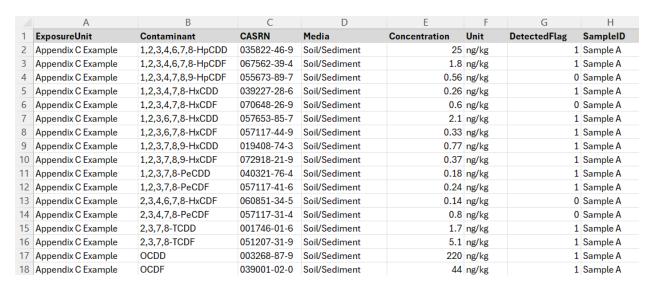
This example demonstrates the preferred approach for calculating TEQs using ATSDR's EPC Tool. The data set considered in this example includes 17 congeners measured in a single soil sample (Helsel, 2010), and are presented in the table below. Health assessors who are using the EPC Tool for the first time are encouraged to replicate this example before using the tool to calculate TEQs for site-specific scenarios. The remainder of this example follows the process outlined in Section 3.0. All figures are screen shots from Excel in Microsoft Office 365TM or the EPC Tool.

Congener Name	Concentration (ng/kg) ^a	
1,2,3,4,6,7,8-HpCDD	25	
1,2,3,4,6,7,8-HpCDF	1.8	
1,2,3,4,7,8,9-HpCDF	<0.56	
1,2,3,4,7,8-HxCDD	0.26	
1,2,3,4,7,8-HxCDF	<0.6	
1,2,3,6,7,8-HxCDD	2.1	
1,2,3,6,7,8-HxCDF	0.33	
1,2,3,7,8,9-HxCDD	0.77	
1,2,3,7,8,9-HxCDF	0.37	
1,2,3,7,8-PeCDD	0.18	
1,2,3,7,8-PeCDF	0.24	
2,3,4,6,7,8-HxCDF	<0.14	
2,3,4,7,8-PeCDF	<0.8	
2,3,7,8-TCDD	1.7	
2,3,7,8-TCDF	5.1	
OCDD	220	
OCDF	44	

Notes:

- a. data as presented in Helsel, D (2010).
- "<" indicates that result was not detected. The value presented is the detection limit.

This information is entered into the EPC Tool Data Import Template as shown below. Importantly, note those congeners that were not detected, denoted with a < symbol in the table above, are entered with only numeric digits in the file and the detection flag set to 0 rather than 1.



Use the "Browse..." button to open a file browser window and select the data import file containing the site information. Note the file cannot be opened on your computer during this process and must be closed. Once the file is selected the "Data Import Summary" will automatically be displayed; however, if there is an error in the data import file a warning will appear.

Instructions: To calculate EPCs:

- 1. Download the Excel data import template by clicking the "Download Data Import Template" link.
- 2. Load your data into the template following the instructions on the template's "ReadMe" tab.
- 3. Click the "Browse" button below and locate the Excel template with your data. A summary table will appear once the data have finished loading.
- 4. Click the Calculate EPC button to calculate EPCs for each unique combination of contaminant, medium, and exposure unit in your dataset.

Upload Data Import Template Browse... AppendixCExample.xlsx

Data Import Summary

Number of Observations	Number of Exposure Units	Number of Contaminants (by CASRN)	Number of Media	Number of EPCs to be Calculated
17	1	17	1	17

Clicking the "Calculate EPC" button will navigate to a new screen where the results are displayed. Note the top entry is the TEQ for the sample and the entries following the TEQ are the individual congeners' EPCs. If the individual congener has its own health guideline value(s) these will be compared against after importing the data into PHAST. To facilitate the subsequent use of the EPC data with PHAST the user needs only to click the "Download PHAST Import Data" button. The "Download All Statistics" button will give a more detailed analysis of the data, which may be useful when more than a single sample is used to generate the EPCs.

