EQUATIONS UTILIZED IN CONJUNCTION WITH SOM02.4

Introduction

This document provides details of equations used in the EPA Contract Laboratory Program (CLP) Statement of Work (SOW) for Organic Superfund Methods (SOM02.4) utilizing values reported in the Staged Electronic Data Deliverable (SEDD). The equations in the SOW use terminology relevant to the particular analytical method, which may or may not be consistent with the terminology used in the SEDD specification. This document defines the SOW equation variables in terms consistent with the location, name, and meaning in the SEDD. Please note that these equations are only applicable to a SEDD Stage 3 file.

> ***The formulas/calculations provided in this document were prepared based on "normal laboratory practices". Any deviations from these "normal laboratory practices" may invalidate these formulas. All CLP contractors must follow their contract requirements, including the SOM02.4 SOW reporting requirements for preparation of a fully compliant Electronic Data Deliverable.***

For each analytical method in Exhibit D of the SOW (Trace Volatiles, Low/Medium Volatiles, Semivolatiles, Pesticides, and Aroclors), the equations are reproduced in the following sections with the same equation number, title, and terms that appear in the SOW. Following the equation, each variable is defined using terminology consistent with the SEDD.

If the result of the equation is reported in the SEDD, this result is defined first by listing the parent node and data element where the result is reported. For example, in EQ. 1 – Relative Response Factor in Exhibit D – Trace Volatiles, "RRF = Peak/RRF" means the result or Equation 1 (RRF) is reported in the SEDD data element "RRF" under the "Peak" node. Figure 1 at the end of this document depicts the SEDD Stage 3 data node hierarchy for reference.

Next, each equation variable is listed in the order in which they appear in the equation and falls into one of three categories: reported in the SEDD, calculated from another equation, or a constant. For example, "Amount Added = Reported Analyte/AmountAdded (µL)" means that the variable "Amount Added" is a value reported in the SEDD and located in the data element "AmountAdded" under the "Analyte" node with units of "µL". The definition "SD_{RRF} = Standard Deviation from EQ. 4" means that the variable "SD_{RRF}" is the result of equation "Standard Deviation" calculated in Equation 4. Constants are represented in the example "V_c = Method required purge volume (25 mL)", where "V_c" is equivalent to "25 mL".

Some SOW equation variables are considered "intermediate results" in the SEDD, which means that they are results based on other equations using values reported in the SEDD. In these cases, sub-equations have been included to derive these intermediate results for inclusion in the SOW equations. These sub-equations are identified by the equation number of the "parent" equation in the SOW with a lowercase letter appended to it (e.g., EQ. 1a, etc.). For example, EQ. 1 – Relative Response Factor in Exhibit D – Trace Volatiles defines the term "C_{is}" as the "Expected Result … from EQ. 1a (ng)." The SOW does not specify how to calculate the Expected Result in ng using values reported in the SEDD; therefore, EQ. 1a is added showing how this result is derived.

Equations for Exhibit D – Trace Volatiles

EQ. 1 Relative Response Factor

$$RRF = \frac{A_x}{A_{is}} \times \frac{C_{is}}{C_x}$$

where,

RRF	=	Peak/RRF.
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
C_{is}	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
C_x	=	Expected Result from EQ. 1a (ng).

EQ. 1a Expected Result

$$\text{Expected Result} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{1000}$$

where,

Expected Result	=	Analyte/ExpectedResult (ng).
Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).

EQ. 2 Mean Value

$$\overline{X} = \frac{\sum_{i=1}^{n} X_i}{n}$$

where,

$\overline{X}$	=	Peak/MeanRRF under the AnalysisGroup node.
X_i	=	Relative Response Factor from EQ. 1 where the reported Analyte/Inclusion is "Yes".
n	=	Number of reported Relative Response Factors where the reported Analyte/Inclusion is "Yes".

EQ. 3 Percent Relative Standard Deviation

$$\%RSD = \frac{SD_{RRF}}{\overline{X}} \times 100$$

where,

%RSD = Peak/PercentRSD under the AnalysisGroup node.

SD_{RRF} = Standard Deviation from EQ. 4.

$\overline{X}$ = Mean RRF from EQ. 2.

EQ. 4 Standard Deviation

$$SD = \sqrt{\frac{\sum_{i=1}^{n} (X_i - \overline{X})^2}{(n-1)}}$$

where,

X_i = Relative Response Factor from EQ. 1 where the reported Analyte/Inclusion is "Yes".

$\overline{X}$ = Mean Relative Response Factor from EQ. 2 where the reported Analyte/Inclusion is "Yes".

n = Number of reported Relative Response Factors where the reported Analyte/Inclusion is "Yes".

EQ. 5 Initial Calibration Verification Percent Difference

$$\%D = \frac{RRF_c - \overline{RRF_i}}{\overline{RRF_i}} \times 100$$

where,

%D = Peak/PercentDifference.

RRF_c = Relative Response Factor from EQ. 1 from the initial calibration verification.

$\overline{RRF_i}$ = Mean Relative Response Factor from EQ. 2.

EQ. 6 Internal Standard Calibration Percent Difference

$$\%D = \frac{RRF_c - \overline{RRF_i}}{\overline{RRF_i}} \times 100$$

where,

%D	=	Peak/PercentDifference.
RRF_c	=	Relative Response Factor from EQ. 1 from the continuing calibration verification.
$\overline{RRF_i}$	=	Mean Relative Response Factor from EQ. 2.

EQ. 7 Water Concentration

$$\text{Concentration } (\mu g/L) = \frac{(A_x)(I_{is})(DF)}{(A_{is})(\overline{RRF})(V_o)}$$

where,

Concentration	=	Analyte/Result.
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
I_{is}	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
$\overline{RRF}$	=	Mean Relative Response Factor from EQ. 2.
DF	=	Reported Analysis/DilutionFactor. Default to 1 for Deuterated Monitoring Compounds.
V_o	=	Reported Analysis/InjectionVolume (mL).

EQ. 8 Water Adjusted CRQL

$$\text{Adjusted CRQL} = \text{Contract CRQL} \times \frac{V_c}{V_o} \times DF$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/L). This is the CRQL value reported in Exhibit C – Table 1 – Trace Volatiles Target Analyte List and Contract Required Quantitation Limits.
V_c	=	Method required purge volume (25 mL).
V_o	=	Reported Analysis/InjectionVolume (mL).
DF	=	Reported Analysis/DilutionFactor.

EQ. 9 DMC Percent Recovery

$$\%R = \frac{Q_d}{Q_a} \times 100$$

where,

%R	=	Analyte/PercentRecovery.
Q_d	=	The Concentration value from EQ. 7 (µg/L).
Q_a	=	The Expected Concentration from EQ. 9a (µg/L).

EQ. 9a Expected Concentration

$$\text{Expected Concentration } (\mu g/L) = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{(1000 \times \text{Injection Volume})}$$

where,

Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).
Injection Volume	=	Reported Analysis/InjectionVolume (mL).

EQ. 10 Matrix Spike Recovery

$$\%R = \frac{SSR - SR}{SA} \times 100$$

where,

%R	=	ReportedResult/PercentRecovery.
SSR	=	The Concentration value from EQ. 7 from the spike sample (µg/L).
SR	=	The Concentration value from EQ. 7 from the original sample (µg/L).
SA	=	Expected Concentration from EQ. 9a from the spike sample (µg/L).

EQ. 11 Relative Percent Difference

$$RPD = \frac{\left|MSR - MSDR\right|}{\frac{1}{2}\left(MSR + MSDR\right)} \times 100$$

where,

RPD	=	ReportedResult/RPD
MSR	=	Matrix Spike Recovery from EQ. 10 from the MS sample.
MSDR	=	Matrix Spike Recovery from EQ. 10 from the MSD sample.

Equations for Exhibit D – Low/Medium Volatiles

EQ. 1 Relative Response Factor

$$RRF = \frac{A_x}{A_{is}} \times \frac{C_{is}}{C_x}$$

where,

RRF	=	Peak/RRF.
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
C_{is}	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
C_x	=	Expected Result from EQ. 1a (ng).

EQ. 1a Expected Result

$$\text{Expected Result} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{1000}$$

where,

Expected Result	=	Analyte/ExpectedResult (ng).
Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).

EQ. 2 Mean Value

$$\overline{X} = \frac{\sum_{i=1}^{n} X_i}{n}$$

where,

$\overline{X}$	=	Peak/MeanRRF under the AnalysisGroup node.
X_i	=	Relative Response Factor from EQ. 1 where the reported Analyte/Inclusion is "Yes".
n	=	Number of reported Relative Response Factors where the reported Analyte/Inclusion is "Yes".

EQ. 3 Percent Relative Standard Deviation

$$\%RSD = \frac{SD_{RRF}}{\overline{X}} \times 100$$

where,

%RSD = Peak/PercentRSD under the AnalysisGroup node.

SD_{RRF} = Standard Deviation from EQ. 4.

$\overline{X}$ = Mean RRF from EQ. 2.

EQ. 4 Standard Deviation

$$SD = \sqrt{\frac{\sum_{i=1}^{n} (X_i - \overline{X})^2}{(n-1)}}$$

where,

X_i = Relative Response Factor from EQ. 1 where the reported Analyte/Inclusion is "Yes".

$\overline{X}$ = Mean Relative Response Factor from EQ. 2 where the reported Analyte/Inclusion is "Yes".

n = Number of reported Relative Response Factors where the reported Analyte/Inclusion is "Yes".

EQ. 5 Initial Calibration Verification Percent Difference

$$\%D = \frac{RRF_c - \overline{RRF_i}}{\overline{RRF_i}} \times 100$$

where,

%D = Peak/PercentDifference.

RRF_c = Relative Response Factor from EQ. 1 from the initial calibration verification.

$\overline{RRF_i}$ = Mean Relative Response Factor from EQ. 2.

EQ. 6 Internal Standard Calibration Percent Difference

$$\%D = \frac{RRF_c - \overline{RRF_i}}{\overline{RRF_i}} \times 100$$

where,

%D	=	Peak/PercentDifference.
RRF_c	=	Relative Response Factor from EQ. 1 from the continuing calibration verification.
$\overline{RRF_i}$	=	Mean Relative Response Factor from EQ. 2.

EQ. 7 Water and TCLP/SPLP Leachate Sample Concentration

$$\text{Concentration } (\mu g/L) = \frac{(A_x)(I_{is})(DF)}{(A_{is})(\overline{RRF})(V_o)}$$

where,

Concentration	=	Analyte/Result.
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
I_{is}	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
$\overline{RRF}$	=	Mean Relative Response Factor from EQ. 2.
DF	=	Reported Analysis/DilutionFactor. Default to 1 for Deuterated Monitoring Compounds.
V_o	=	Reported Analysis/InjectionVolume (mL).

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated concentration by 1000.

EQ. 8 Low-Level Soil/Sediment Concentration

$$\text{Concentration } (\mu g/kg) = \frac{(A_x)(I_{is})(DF)}{(A_{is})(\overline{RRF})(W_s)(S)}$$

where,

Concentration	=	Analyte/Result.
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
I_{is}	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).

$\overline{RRF}$ = Mean Relative Response Factor from EQ. 2.

DF = Reported Analysis/DilutionFactor. Default to 1 for Deuterated Monitoring Compounds.

W_s = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).

S = (Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

EQ. 9 Medium-Level Soil/Sediment Concentration

$$\text{Concentration } (\mu g/kg) = \frac{(A_x)(I_{is})(AV_t)(1000)(DF)}{(A_{is})(\overline{RRF})(V_a)(W_s)(S)}$$

where,

Concentration = Analyte/Result.

A_x = Reported Peak/Response.

A_{is} = Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.

I_{is} = Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).

$\overline{RRF}$ = Mean Relative Response Factor from EQ. 2.

AV_t = Adjusted Total Volume from EQ. 9a (µL).

V_a = Reported Analysis/AnalyzedAmount (µL).

DF = Reported Analysis/DilutionFactor. Default to 1 for Deuterated Monitoring Compounds.

W_s = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).

S = (Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

EQ. 9a Adjusted Total Volume

$$AV_t = V_t + \left[W_s - (W_s \times S)\right]$$

where,

AV_t = Adjusted Total Volume (µL).

V_t = Reported PreparationPlusCleanup/InitialAmount from the preparation node (µL).

W_s = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).

S = (Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

EQ. 10 Water and TCLP/SPLP Leachate Sample Adjusted CRQL

$$\text{Adjusted CRQL} = \text{Contract CRQL} \times \frac{V_c}{V_o} \times \text{DF}$$

where,

Adjusted CRQL = ReportedResult/QuantitationLimit (µg/L).

Contract CRQL = ReportedResult/ClientQuantitationLimit (µg/L). This is the CRQL value reported in Exhibit C – Table 2 – Low/Medium Volatiles Target Analyte List and Contract Required Quantitation Limits.

V_c = Method required purge volume (5 mL).

V_o = Reported Analysis/InjectionVolume (mL).

DF = Reported Analysis/DilutionFactor.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated CRQL by 1000.

EQ. 11 Low-Level Soil Adjusted CRQL

$$\text{Adjusted CRQL} = \text{Contract CRQL} \times \frac{(W_c)}{(W_s)\ (S)}$$

where,

Adjusted CRQL = ReportedResult/QuantitationLimit (µg/kg).

Contract CRQL = ReportedResult/ClientQuantitationLimit (µg/kg). This is the CRQL value reported in Exhibit C – Table 2 – Low/Medium Volatiles Target Analyte List and Contract Required Quantitation Limits.

W_c = Method required sample weight (5.0 g).

W_s = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).

S = (Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

EQ. 12 Medium-Level Soil/Sediment Adjusted CRQL

$$\text{Adjusted CRQL} = \text{Contract CRQL} \times \frac{(W_x)(AV_t)(V_y)(1000)(DF)}{(W_s)(V_c)(V_a)(S)}$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/kg). This is the CRQL value reported in Exhibit C – Table 2 – Low/Medium Volatiles Target Analyte List and Contract Required Quantitation Limits.
W_x	=	Method required sample weight (5.0 g).
W_s	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
AV_t	=	Adjusted Total Volume from EQ. 9a (µL).
V_c	=	Method required soil methanol extract volume (5000 µL).
V_y	=	Method required soil aliquot volume (100 µL).
V_a	=	Reported Analysis/AnalyzedAmount (µL).
DF	=	Reported Analysis/DilutionFactor.
S	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

EQ. 13 DMC Percent Recovery

$$\%R = \frac{Q_d}{Q_a} \times 100$$

where,

%R	=	Analyte/PercentRecovery.
Q_d	=	Concentration value from EQ. 7, 8, or 9 (µg/L or µg/kg).
Q_a	=	Expected Concentration from EQ. 13a (µg/L or µg/kg).

EQ. 13a Expected Concentration

$$\text{Expected Concentration (µg/L or µg/kg)} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{(1000 \times \text{Aliquot Amount} \times \text{Solids Factor})}$$

where,

Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).
Aliquot Amount	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node for soil/sediment samples, or Analysis/InjectionVolume for water samples (g or mL).
Solids Factor	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation and water samples.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated concentration by 1000.

EQ. 14 Matrix Spike Recovery

$$\%R = \frac{SSR - SR}{SA} \times 100$$

where,

%R	=	ReportedResult/PercentRecovery.
SSR	=	The Concentration value from EQ. 7, 8, or 9 from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 7, 8, or 9 from the original sample (µg/L or µg/kg).
SA	=	Expected Concentration from EQ. 13a from the spike sample (µg/L or µg/kg).

EQ. 15 Relative Percent Difference

$$RPD = \frac{|MSR - MSDR|}{\frac{1}{2}(MSR + MSDR)} \times 100$$

where,

RPD	=	ReportedResult/RPD.
MSR	=	Matrix Spike Recovery from EQ. 14 from the MS sample.
MSDR	=	Matrix Spike Recovery from EQ. 14 from the MSD sample.

Equations for Exhibit D – Semivolatiles

EQ. 1 Relative Response Factor

$$RRF = \frac{A_x}{A_{is}} \times \frac{C_{is}}{C_x}$$

where,

RRF	=	Peak/RRF.
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
C_{is}	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
C_x	=	Expected Result from EQ. 1a (ng).

EQ. 1a Expected Result

$$\text{Expected Result} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{1000} + C_{os}$$

where,

Expected Result	=	Analyte/ExpectedResult (ng).
Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).
C_{os}	=	Internal Standard Original Sample Expected Result from EQ. 1b for dilutions or reinjections prepared from a sample to which internal standards have been added identified by the Analysis/OriginalLabAnalysisID element (ng). Default to 0 for samples not prepared from a sample to which internal standards have been added.

EQ. 1b Internal Standard Original Sample Expected Result

$$C_{os} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{1000} \times \frac{DF}{DF_{os}}$$

where,

Standard Concentration	=	Reported Analyte/StandardConcentration of the associated internal standard in the original sample identified by the Analysis/OriginalLabAnalysisID element (µg/L).
Amount Added	=	Reported Analyte/AmountAdded of the associated internal standard in the original sample identified by the Analysis/OriginalLabAnalysisID element (µL).

DF = Reported Analysis/DilutionFactor.

DF_{os} = Reported Analysis/DilutionFactor of the original sample analysis identified by the Analysis/OriginalLabAnalysisID element.

EQ. 2 Mean Value

$$\overline{X} = \frac{\sum_{i=1}^{n} X_i}{n}$$

where,

$\overline{X}$ = Peak/MeanRRF under the AnalysisGroup node.

X_i = Relative Response Factor from EQ. 1 where the reported Analyte/Inclusion is "Yes".

n = Number of reported Relative Response Factors where the reported Analyte/Inclusion is "Yes".

EQ. 3 Percent Relative Standard Deviation

$$\%RSD = \frac{SD_{RRF}}{\overline{X}} \times 100$$

where,

$\%RSD$ = Peak/PercentRSD under the AnalysisGroup node.

SD_{RRF} = Standard Deviation from EQ. 4.

$\overline{X}$ = Mean RRF from EQ. 2.

EQ. 4 Standard Deviation

$$SD = \sqrt{\frac{\sum_{i=1}^{n} (X_i - \overline{X})^2}{(n-1)}}$$

where,

X_i = Relative Response Factor from EQ. 1 where the reported Analyte/Inclusion is "Yes".

$\overline{X}$ = Mean Relative Response Factor from EQ. 2 where the reported Analyte/Inclusion is "Yes".

n = Number of reported Relative Response Factors where the reported Analyte/Inclusion is "Yes".

EQ. 5 Initial Calibration Verification Percent Difference

$$\%D = \frac{RRF_c - \overline{RRF_i}}{\overline{RRF_i}} \times 100$$

where,

%D	=	Peak/PercentDifference.
RRF_c	=	Relative Response Factor from EQ. 1 from the initial calibration verification.
$\overline{RRF_i}$	=	Mean Relative Response Factor from EQ. 2.

EQ. 6 Internal Standard Calibration Percent Difference

$$\%D = \frac{RRF_c - \overline{RRF_i}}{\overline{RRF_i}} \times 100$$

where,

%D	=	Peak/PercentDifference.
RRF_c	=	Relative Response Factor from EQ. 1 from the continuing calibration verification.
$\overline{RRF_i}$	=	Mean Relative Response Factor from EQ. 2.

EQ. 7 Water and TCLP/SPLP Leachate Sample Concentration

$$\text{Concentration } (\mu g/L) = \left(\frac{A_x \times I_{is}}{A_{is} \times \overline{RRF}}\right)\left(\frac{DF}{V_i}\right)\left(\frac{V_t}{V_o}\right)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Concentration	=	Analyte/Result.
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
I_{is}	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
$\overline{RRF}$	=	Mean Relative Response Factor from EQ. 2.
DF	=	Reported Analysis/DilutionFactor.
V_o	=	Reported PreparationPlusCleanup/AliquotAmount (mL).
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).
V_i	=	Reported Analysis/InjectionVolume (µL).

CV_{out} = Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).

CV_{in} = Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).

E = Reported PreparationPlusCleanup/Efficiency from each cleanup node.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated concentration by 1000.

EQ. 8 Soil/Sediment Concentration

$$\text{Concentration } (\mu g/kg) = \left(\frac{A_x \times I_{is}}{A_{is} \times \overline{RRF}}\right)\left(\frac{DF}{V_i}\right)\left(\frac{V_t}{W_t \times S}\right)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Concentration = Analyte/Result.

A_x = Reported Peak/Response.

A_{is} = Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.

I_{is} = Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).

$\overline{RRF}$ = Mean Relative Response Factor from EQ. 2.

DF = Reported Analysis/DilutionFactor.

V_i = Reported Analysis/InjectionVolume (µL).

V_t = Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).

W_t = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).

S = (Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

CV_{out} = Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).

CV_{in} = Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).

E = Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 9 Water and TCLP/SPLP Leachate Sample Adjusted CRQL

$$\text{Adjusted CRQL} = (\text{Contract CRQL}) \left(\frac{V_x}{V_o}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in}\times E}\right)_1\left(\frac{CV_{out}}{CV_{in}\times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in}\times E}\right)_n$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/L). This is the CRQL value reported in Exhibit C – Table 3 – Semivolatiles Target Analyte List and Contract Required Quantitation Limits.
V_x	=	Method required sample volume (1000 mL).
V_o	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL).
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).
V_y	=	Method required concentrated extract volume (1000 µL).
DF	=	Reported Analysis/DilutionFactor.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated CRQL by 1000.

EQ. 10 Soil/Sediment Adjusted CRQL

$$\text{Adjusted CRQL} = (\text{Contract CRQL}) \left(\frac{W_x}{W_t\times S}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in}\times E}\right)_1\left(\frac{CV_{out}}{CV_{in}\times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in}\times E}\right)_n$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/kg). This is the CRQL value reported in Exhibit C – Table 3 – Semivolatiles Target Analyte List and Contract Required Quantitation Limits.
W_x	=	Contract sample weight (30 g for low-level soil/sediment samples and 1.0 g for medium-level soil/sediment samples).
W_t	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).

S	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).
V_y	=	Contract concentrated extract volume (1000 µL).
DF	=	Reported Analysis/DilutionFactor.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 11 DMC Percent Recovery

$$\%R = \frac{Q_d \times DF}{Q_a} \times 100$$

where,

%R	=	Analyte/PercentRecovery.
Q_d	=	The Concentration value from EQ. 7 or 8 (µg/L or µg/kg).
Q_a	=	Expected Concentration from EQ. 11a (µg/L or µg/kg).
DF	=	Not used because the dilution factor is already accounted for in the Q_d term.

EQ. 11a Expected Concentration

$$\text{Expected Concentration (µg/L or µg/kg)} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{(1000 \times \text{Aliquot Amount} \times \text{Solids Factor})}$$

where,

Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).
Aliquot Amount	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL or g).
Solids Factor	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples and water samples.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated concentration by 1000.

EQ. 12 Matrix Spike Recovery

$$\%R = \frac{SSR - SR}{SA} \times 100$$

where,

%R	=	ReportedResult/PercentRecovery.
SSR	=	The Concentration value from EQ. 7 or 8 from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 7 or 8 from the original sample (µg/L or µg/kg).
SA	=	Expected Concentration from EQ. 11a from the spike sample (µg/L or µg/kg).

EQ. 13 Relative Percent Difference

$$RPD = \frac{\left|MSR - MSDR\right|}{\frac{1}{2}\left(MSR + MSDR\right)} \times 100$$

where,

RPD	=	ReportedResult/RPD.
MSR	=	Matrix Spike Recovery from EQ. 12 from the MS sample.
MSDR	=	Matrix Spike Recovery from EQ. 12 from the MSD sample.

Equations for Exhibit D – Pesticides

EQ. 1 Percent Resolution

$$\% \text{ Resolution} = \frac{V}{H} \times 100$$

where,

V = Depth of the valley between the two peaks. The depth of the valley is measured along a vertical line from the level of the apex of the shorter peak to the floor of the valley between the two peaks.

H = Height of the shorter of the adjacent peaks.

This equation is not calculated from the SEDD. This result is reported in the element Peak/Resolution.

EQ. 2 Mean Retention Time

$$\overline{RT} = \frac{\sum_{i=1}^{n} RT_i}{n}$$

where,

$\overline{RT}$ = Peak/MeanRetentionTime under the AnalysisGroup node.

RT_i = Reported Peak/RetentionTime where the reported Analyte/Inclusion is "Yes".

n = Number of reported RetentionTime values where the reported Analyte/Inclusion is "Yes".

EQ. 3 Calibration Factor

$$CF = \frac{\text{Peak area (or peak height) of the standard}}{\text{Mass Injected (ng)}}$$

where,

CF = Peak/CalibrationFactor.

Peak area (or peak height) of the standard = Reported Peak/Response.

Mass Injected (ng) = Expected Intermediate Result from EQ. 3a (ng).

EQ. 3a Expected Intermediate Result

$$\text{Expected Intermediate Result (ng)} = \frac{(\text{Standard Concentration} \times \text{Injection Volume} \times \text{Amount Added})}{(\text{Analyzed Amount} \times 1000)}$$

where,

Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Injection Volume	=	Reported Analysis/InjectionVolume (µL).
Amount Added	=	Reported Analyte/AmountAdded (µL).
Analyzed Amount	=	Reported Analysis/AnalyzedAmount (µL).

EQ. 4 Mean Calibration Factor

$$\overline{CF} = \frac{\sum_{i=1}^{n} CF_i}{n}$$

where,

$\overline{CF}$	=	Peak/MeanCalibrationFactor under the AnalysisGroup node.
CF_i	=	Calibration Factor from EQ. 3 where the reported Analyte/Inclusion is "Yes".
n	=	Number of reported Calibration Factors where the reported Analyte/Inclusion is "Yes".

EQ. 5 Standard Deviation of Calibration Factors

$$SD_{CF} = \sqrt{\frac{\sum_{i=1}^{n} \left(CF_i - \overline{CF}\right)^2}{(n-1)}}$$

where,

CF_i	=	Calibration Factor from EQ. 3 where the reported Analyte/Inclusion is "Yes".
$\overline{CF}$	=	Mean Calibration Factor from EQ. 4.
n	=	Number of reported Calibration Factors where the reported Analyte/Inclusion is "Yes".

EQ. 6 Percent Relative Standard Deviation of the Calibration Factors

$$\%\text{RSD} = \frac{\text{SD}_{\text{CF}}}{\overline{\text{CF}}} \times 100$$

where,

%RSD	=	Peak/PercentRSD under the AnalysisGroup node.
SD_{CF}	=	Standard Deviation of the Calibration Factors from EQ. 5.
$\overline{\text{CF}}$	=	Mean Calibration Factor from EQ. 4.

EQ. 7 Amount Found

$$\text{Amount found (ng)} = \frac{\text{Peak area (or peak height) of compound in PEM}}{\overline{\text{CF}}}$$

where,

Amount found	=	Peak/IntermediateResult.
Peak area (or peak height) of compound in PEM	=	Reported Peak/Response.
$\overline{\text{CF}}$	=	Mean Calibration Factor from EQ. 4.

EQ. 8 Percent Breakdown of DDT

$$\%\text{Breakdown DDT} = \frac{\text{Amount found (ng) (DDD + DDE)}}{\text{Amount (ng) of DDT injected}} \times 100$$

where,

%Breakdown DDT	=	Analyte/PercentBreakdown.
Amount found (ng) (DDD + DDE)	=	(Amount Found of DDD + Amount Found of DDE) from EQ. 7 (ng).
Amount (ng) of DDT injected	=	Expected Intermediate Result of DDT from EQ. 3a (ng).

EQ. 9 Percent Breakdown of Endrin

$$\%\text{Breakdown Endrin} = \frac{\text{Amount found (ng) (Endrin Aldehyde + Endrin Ketone)}}{\text{Amount (ng) of Endrin injected}} \times 100$$

where,

%Breakdown Endrin	=	Analyte/PercentBreakdown.
Amount found (ng) (Endrin Aldehyde + Eldrin Ketone)	=	Amount Found of Endrin Aldehyde + Endrin Ketone from EQ. 7 (ng).
Amount (ng) of Endrin injected	=	Expected Intermediate Result of Endrin from EQ. 3a (ng).

EQ. 10 Combined Percent Breakdown of DDT and Endrin

$$\text{Combined \%Breakdown} = \text{\%Breakdown DDT} + \text{\%Breakdown Endrin}$$

where,

%Breakdown DDT	=	Percent Breakdown of DDT from EQ. 8.
%Breakdown Endrin	=	Percent Breakdown of Endrin from EQ. 9.

EQ. 11 Percent Difference Between the Calculated and Nominal Amount

$$\%D = \frac{(C_{calc} - C_{nom})}{C_{nom}} \times 100$$

where,

%D	=	Peak/PercentDifference.
C_{calc}	=	Amount Found from EQ. 7 (ng).
C_{nom}	=	Expected Intermediate Result from EQ. 3a (ng).

EQ. 12 External Standard Calibration Percent Difference

$$\%D = \frac{CF - \overline{CF}}{\overline{CF}} \times 100$$

where,

%D	=	Peak/PercentDifference.
CF	=	Calibration Factor from EQ. 3.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 4.

EQ. 13 Percent Recovery

$$\%R = \frac{(Q_d \times DF)}{Q_a} \times 100$$

where,

%R	=	Analyte/PercentRecovery.
Q_d	=	Intermediate Result from EQ. 13a (ng).
Q_a	=	Theoretical Intermediate Result from EQ. 13b (ng).
DF	=	Not used because the dilution factor is already accounted for in the Q_a term from EQ. 13b.

EQ. 13a Intermediate Result

$$\text{Intermediate Result} = \frac{\sum_{i=1}^{n} (\text{Amount Found})}{n}$$

where,

Intermediate Result	=	Analyte/IntermediateResult (ng).
Amount Found	=	Amount Found from EQ. 7 (ng).
n	=	Number of non-missing Amount Found values.

EQ. 13b Theoretical Intermediate Result

$$\text{Theoretical Intermediate Result (ng)} = \frac{(\text{Expected Result} \times \text{Cleanup Factor} \times \text{Injection Volume})}{(\text{Prep Final Amount} \times \text{Dilution Factor} \times \text{Cleanup Initial Amount})}$$

where,

Expected Result	=	Expected Result from EQ. 13c (ng).
Cleanup Factor	=	Cleanup Factor from EQ. 13d. Default to 1 for instrument blanks or if cleanup is not performed.
Injection Volume	=	Reported Analysis/InjectionVolume (µL).
Prep Final Amount	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL). Default to 10,000 for instrument blanks, 1000 for florisil cartridge performance checks, and 1 for GPC Calibration Checks and Cleanup Blanks.
Dilution Factor	=	Reported Analysis/DilutionFactor.
Cleanup Initial Amount	=	Reported PreparationPlusCleanup/InitialAmount from the cleanup node for GPC Calibration Checks and Cleanup Blanks (µL). Default to 1 for all other analyses.

EQ. 13c Expected Result

$$\text{Expected Result} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{1000}$$

where,

Expected Result	=	Analyte/ExpectedResult (ng).
Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).

EQ. 13d Cleanup Factor

$$\text{Cleanup Factor} = \left(\frac{\text{Initial Amount} \times \text{E}}{\text{Final Amount}}\right)_1 \left(\frac{\text{Initial Amount} \times \text{E}}{\text{Final Amount}}\right)_2 \cdots \left(\frac{\text{Initial Amount} \times \text{E}}{\text{Final Amount}}\right)_n$$

where,

Initial Amount	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
Final Amount	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 14 Water and TCLP/SPLP Leachate Sample Concentration

$$\text{Concentration (µg/L)} = \left(\frac{A_x}{\overline{CF}}\right)\left(\frac{DF}{V_i}\right)\left(\frac{V_t}{V_o}\right)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1 \left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Concentration	=	Analyte/Result. For toxaphene, individual peak results will be averaged to yield the final analyte result.
A_x	=	Reported Peak/Response.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 4.
DF	=	Reported Analysis/DilutionFactor.
V_i	=	Reported Analysis/InjectionVolume (µL).
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL). Default to 10,000 for instrument blanks and 1000 for florisil cartridge performance checks.
V_o	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL). Default to 1000 for instrument and sulfur blanks.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated concentration by 1000.

EQ. 15 On-Column Concentration

$$\text{On-Column Concentration } (ng/\mu L) = \frac{(A_x)}{(\overline{CF})(V_i)}$$

where,

A_x = Reported Peak/Response.

$\overline{CF}$ = Mean Calibration Factor from EQ. 4.

V_i = Reported Analysis/InjectionVolume (µL).

EQ. 16 Soil/Sediment Concentration

$$\text{Concentration } (\mu g/kg) = \left(\frac{A_x}{\overline{CF}}\right)\left(\frac{DF}{V_i}\right)\left(\frac{V_t}{W_t \times S}\right)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Concentration = Analyte/Result. For toxaphene, individual peak results will be averaged to yield the final analyte result.

A_x = Reported Peak/Response.

$\overline{CF}$ = Mean Calibration Factor from EQ. 4.

DF = Reported Analysis/DilutionFactor.

V_i = Reported Analysis/InjectionVolume (µL).

V_t = Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).

W_t = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).

S = (Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

CV_{out} = Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).

CV_{in} = Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).

E = Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 17 Percent Difference Between Concentrations on Both GC Columns

$$\%D = \frac{Conc_H - Conc_L}{Conc_L} \times 100$$

where,

%D	=	ReportedResult/PercentDifference.
$Conc_H$	=	The greater of the Concentration values from EQ. 14 or 16 from the two Analysis nodes where the analyte is detected on both GC columns (µg/L or µg/kg).
$Conc_L$	=	The lesser of the Concentration values from EQ. 14 or 16 from the two Analysis nodes where the analyte is detected on both GC columns (µg/L or µg/kg).

EQ. 18 Water and TCLP/SPLP Leachate Sample Adjusted CRQL

$$\text{Adjusted CRQL} = (\text{Contract CRQL}) \left(\frac{V_x}{V_o}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/L). This is the CRQL value reported in Exhibit C – Table 4 – Pesticides Target Analyte List and Contract Required Quantitation Limits.
V_x	=	Method required sample volume (1000 mL).
V_o	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL). Default to 1000 for instrument blanks.
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL). Default to 10,000 for instrument and sulfur blanks.
V_y	=	Method required concentrated extract volume (10,000 µL).
DF	=	Reported Analysis/DilutionFactor.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated CRQL by 1000.

EQ. 19 Soil/Sediment Adjusted CRQL

$$\text{Adjusted CRQL} = (\text{Contract CRQL}) \left(\frac{W_x}{W_t \times S}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1 \left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/kg). This is the CRQL value reported in Exhibit C – Table 4 – Pesticides Target Analyte List and Contract Required Quantitation Limits.
W_x	=	Method required sample weight (30 g).
W_t	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
S	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).
V_y	=	Method required concentrated extract volume (10,000 µL).
DF	=	Reported Analysis/DilutionFactor.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 20 Matrix Spike Recovery

$$\%R = \frac{SSR - SR}{SA} \times 100$$

where,

%R	=	ReportedResult/PercentRecovery.
SSR	=	The Concentration value from EQ. 14 or 16 from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 14 or 16 from the original sample (µg/L or µg/kg).
SA	=	The Expected Concentration from EQ. 20a from the spike sample (µg/L or µg/kg).

This equation is also used for calculating percent recovery for LCS.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated concentration by 1000.

EQ. 20a Expected Concentration

$$\text{Expected Concentration} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{(1000 \times \text{Aliquot Amount} \times \text{Solids Factor})}$$

where,

Expected Concentration	=	Analyte/ExpectedResult (µg/L or µg/kg).
Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).
Aliquot Amount	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL or g).
Solids Factor	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for water samples and Performance Evaluation samples.

Note: Convert units to mg/L for TCLP leachates by dividing the final calculated concentration by 1000.

EQ. 21 Relative Percent Difference

$$\text{RPD} = \frac{\left|\text{MSR} - \text{MSDR}\right|}{\frac{1}{2}\left(\text{MSR} + \text{MSDR}\right)} \times 100$$

where,

RPD	=	ReportedResult/RPD.
MSR	=	Matrix Spike Recovery from EQ. 20 from the MS sample.
MSDR	=	Matrix Spike Recovery from EQ. 20 from the MSD sample.

Equations for Exhibit D – Aroclors

EQ. 1 Mean Retention Time

$$\overline{RT} = \frac{\sum_{i=1}^{n} RT_i}{n}$$

where,

$\overline{RT}$	=	Peak/MeanRetentionTime under the AnalysisGroup node.
RT_i	=	Reported Peak/RetentionTime where the reported Analyte/Inclusion is "Yes".
n	=	Number of reported RetentionTime values where the Analyte/Inclusion is "Yes".

EQ. 2 Calibration Factor

$$CF = \frac{\text{Peak area (or peak height) of the standard}}{\text{Mass Injected (ng)}}$$

where,

CF	=	Peak/CalibrationFactor.
Peak area (or peak height) of the standard	=	Reported Peak/Response.
Mass Injected (ng)	=	Expected Intermediate Result from EQ. 2a (ng).

EQ. 2a Expected Intermediate Result

$$\text{Expected Intermediate Result} = \frac{(\text{Standard Concentration} \times \text{Injection Volume} \times \text{Amount Added})}{(\text{Analyzed Amount} \times 1000)}$$

where,

Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Injection Volume	=	Reported Analysis/InjectionVolume (µL).
Amount Added	=	Reported Analyte/AmountAdded (µL).
Analyzed Amount	=	Reported Analysis/AnalyzedAmount (µL).

EQ. 3 Mean Calibration Factor

$$\overline{CF} = \frac{\sum_{i=1}^{n} CF_i}{n}$$

where,

$\overline{CF}$ = Peak/MeanCalibrationFactor under the AnalysisGroup node.

CF_i = Calibration Factor from EQ. 2 where the reported Analyte/Inclusion is "Yes".

n = Number of reported Calibration Factors where the reported Analyte/Inclusion is "Yes".

EQ. 4 Standard Deviation of Calibration Factors

$$SD_{CF} = \sqrt{\frac{\sum_{i=1}^{n}\left(CF_i - \overline{CF}\right)^2}{(n-1)}}$$

where,

CF_i = Calibration Factor from EQ. 2 where the reported Analyte/Inclusion is "Yes".

$\overline{CF}$ = Mean Calibration Factor from EQ. 3.

n = Number of reported Calibration Factors where the reported Analyte/Inclusion is "Yes".

EQ. 5 Percent Relative Standard Deviation of the Calibration Factors

$$\%RSD = \frac{SD_{CF}}{\overline{CF}} \times 100$$

where,

%RSD = Peak/PercentRSD under the AnalysisGroup node.

SD_{CF} = Standard Deviation of the Calibration Factors from EQ. 4.

$\overline{CF}$ = Mean Calibration Factor from EQ. 3.

EQ. 6 External Standard Calibration Percent Difference

$$\%D = \frac{CF - \overline{CF}}{\overline{CF}} \times 100$$

where,

%D = Peak/PercentDifference.

CF = Calibration Factor from EQ. 2.

$\overline{CF}$ = Mean Calibration Factor from EQ. 3.

EQ. 7 Water Concentration

$$\text{Concentration } (\mu g/L) = \left(\frac{A_x}{\overline{CF}}\right)\left(\frac{DF}{V_i}\right)\left(\frac{V_t}{V_o}\right)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Concentration	=	Analyte/Result. Individual peak results will be averaged to yield the final analyte result.
A_x	=	Reported Peak/Response.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 3.
DF	=	Reported Analysis/DilutionFactor.
V_i	=	Reported Analysis/InjectionVolume (µL).
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL). Default to 10,000 for instrument blanks.
V_o	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL). Default to 1000 for instrument blanks.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 8 On-Column Concentration

$$\text{On-Column Concentration } (ng/\mu L) = \frac{(A_x)}{(\overline{CF})(V_i)}$$

where,

A_x	=	Reported Peak/Response.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 3.
V_i	=	Reported Analysis/InjectionVolume (µL).

EQ. 9 Soil/Sediment Concentration

$$\text{Concentration } (\mu g/kg) = \left(\frac{A_x}{\overline{CF}}\right)\left(\frac{DF}{V_i}\right)\left(\frac{V_t}{W_t \times S}\right)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Concentration	=	Analyte/Result. Individual peak results will be averaged to yield the final analyte result.
A_x	=	Reported Peak/Response.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 3.
DF	=	Reported Analysis/DilutionFactor.
V_i	=	Reported Analysis/InjectionVolume (µL).
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).
W_t	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
S	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 10 Percent Difference

$$\%D = \frac{Conc_H - Conc_L}{Conc_L} \times 100$$

where,

%D	=	ReportedResult/PercentDifference.
$Conc_H$	=	The greater of the Concentration values from EQ. 7 or 9 from the two Analysis nodes where the analyte is detected on both GC columns (µg/L or µg/kg).
$Conc_L$	=	The lesser of the Concentration values from EQ. 7 or 9 from the two Analysis nodes where the analyte is detected on both GC columns (µg/L or µg/kg).

EQ. 11 Water Adjusted CRQL

$$\text{Adjusted CRQL} = (\text{Contract CRQL}) \left(\frac{V_x}{V_o}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/L). This is the CRQL value reported in Exhibit C – Table 5 – Aroclors Target Analyte List and Contract Required Quantitation Limits.
V_x	=	Method required sample volume (1000 mL).
V_o	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL). Default to 1000 for instrument blanks.
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL). Default to 10,000 for instrument blanks.
V_y	=	Method required concentrated extract volume (10,000 µL).
DF	=	Reported Analysis/DilutionFactor.
CV_{out}	=	Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).
CV_{in}	=	Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).
E	=	Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 12 Soil/Sediment Adjusted CRQL

$$\text{Adjusted CRQL} = (\text{Contract CRQL}) \left(\frac{W_x}{W_t \times S}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_n$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	ReportedResult/ClientQuantitationLimit (µg/kg). This is the CRQL value reported in Exhibit C – Table 5 – Aroclors Target Analyte List and Contract Required Quantitation Limits.
W_x	=	Method required sample weight (30 g).
W_t	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
S	=	(Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for Performance Evaluation samples.

V_t = Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).

V_y = Method required concentrated extract volume (10,000 µL).

DF = Reported Analysis/DilutionFactor.

CV_{out} = Reported PreparationPlusCleanup/FinalAmount from each cleanup node (µL).

CV_{in} = Reported PreparationPlusCleanup/InitialAmount from each cleanup node (µL).

E = Reported PreparationPlusCleanup/Efficiency from each cleanup node.

EQ. 13 Surrogate Recovery

$$\%R = \frac{(Q_d \times DF)}{Q_a} \times 100$$

where,

%R = Analyte/PercentRecovery.

Q_d = The Concentration value from EQ. 7 or 9.

Q_a = Expected Concentration from EQ. 13a (µg/L or µg/kg).

DF = Not used because the dilution factor is already accounted for in the Q_d term.

EQ. 13a Expected Concentration

$$\text{Expected Concentration} = \frac{(\text{Standard Concentration} \times \text{Amount Added})}{(1000 \times \text{Aliquot Amount} \times \text{Solids Factor})}$$

where,

Expected Concentration = Analyte/ExpectedResult (µg/L or µg/kg).

Standard Concentration = Reported Analyte/StandardConcentration (µg/L).

Amount Added = Reported Analyte/AmountAdded (µL).

Aliquot Amount = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL or g).

Solids Factor = (Characteristic/CharacteristicValue ÷ 100) from the Characteristic node with Characteristic/CharacteristicType = "Percent_Solids". Default to 1 for water samples and Performance Evaluation samples.

EQ. 14 Matrix Spike Recovery

$$\%R = \frac{SSR - SR}{SA} \times 100$$

where,

%R	=	ReportedResult/PercentRecovery.
SSR	=	The Concentration value from EQ. 7 or 9 from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 7 or 9 from the original sample (µg/L or µg/kg).
SA	=	Expected Concentration from EQ. 13a from the spike sample (µg/L or µg/kg).

This equation is also used for calculating percent recovery for LCS.

EQ. 15 Relative Percent Difference

$$RPD = \frac{\left|MSR - MSDR\right|}{\frac{1}{2}\left(MSR + MSDR\right)} \times 100$$

where,

RPD	=	ReportedResult/RPD.
MSR	=	Matrix Spike Recovery from EQ. 14 from the MS sample.
MSDR	=	Matrix Spike Recovery from EQ. 14 from the MSD sample.

Figure 1: SEDD Stage 3 Data Node Hierarchy