EQUATIONS UTILIZED IN CONJUNCTION WITH SOM01.2

AUGUST 22, 2007

Introduction

This document provides details of equations used in the Contract Laboratory Program Analytical Methods for Organic Analysis (SOM01.2) statement of work (SOW) 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.

> ***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 SOM01.2 Statement of Work 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 and title 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 Calculation 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 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. 3" means that the variable "SD_{RRF}" is the result of equation "Standard Deviation" calculated in Equation 3. Constants are represented in the example "V_c = Contract sample volume (25 mL)" where "V_c" is equivalent to "25 mL".

Some SOW equation variables are considered "intermediate results" in SEDD, which means 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. 8a, EQ. 8b, EQ. 8c, etc.). For example, EQ. 1 - Relative Response Factor Calculation 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 Calculation

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

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 Percent Relative Standard Deviation Calculation

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

where,

%RSD	=	Peak/PercentRSD under the AnalysisGroup node.
SD_{RRF}	=	Standard Deviation from EQ. 3.
$\overline{X}$	=	Mean RRF from EQ. 4.

EQ. 3 Standard Deviation Calculation

$$\text{Standard Deviation} = \sqrt{\frac{\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}{\left(n-1\right)}}$$

where,

x_i = Relative Response Factor from EQ. 1 where the reported Peak/RRF is not null.

$\bar{x}$ = Mean Relative Response Factor from EQ. 4 where the reported Peak/RRF is not null.

n = Number of non-missing Relative Response Factor values.

EQ. 4 Mean Value Calculation

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

where,

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

X_i = Relative Response Factor EQ. 1 where the reported Peak/RRF is not null.

n = Number of non-missing Relative Response Factor values.

EQ. 5 Relative Response Factor Percent Difference Calculation

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

where,

$\%\text{Difference}_{RRF}$ = Peak/PercentDifference.

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

$\overline{RRF_i}$ = Mean Relative Response Factor from EQ. 4.

EQ. 6 Water Concentration Calculation

$$\text{Concentration in } \mu g/L = \left(\frac{A_x \times I_s}{A_{is} \times \overline{RRF}}\right)\left(\frac{DF}{V_o}\right)$$

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_s	=	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. 4.
DF	=	Reported Analysis/DilutionFactor. Default to 1 for deuterated monitoring compounds.
V_o	=	Reported Analysis/InjectionVolume (mL).

EQ. 7 Water Adjusted CRQL Calculation

$$\text{Adjusted CRQL} = (\text{Contract CRQL})\left(\frac{V_c}{V_o}\right)(\text{DF})$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	The CRQL value reported in Exhibit C –Volatiles (µg/L).
V_c	=	Contract sample volume (25 mL).
V_o	=	Reported Analysis/InjectionVolume (mL).
DF	=	Reported Analysis/DilutionFactor.

EQ. 8 DMC Percent Recovery Calculation

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

where,

%R	=	Analyte/PercentRecovery.
Q_d	=	Intermediate Result from EQ. 8a (ng).
Q_a	=	Theoretical Intermediate Result from EQ. 8b (ng).

Note: EQ. 8 in the SOM01.1 SOW contains the term DF (Dilution Factor) in the numerator. EXES does not use this value because dilution factor is accounted for in the term Qa (Theoretical Intermediate Result) in EQ. 8b.

EQ. 8a Intermediate Result

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

where,

Amount Found	=	Amount Found from EQ 8c (ng).
n	=	Number of non-missing Amount Found values.

EQ. 8b Theoretical Intermediate Result

$$\text{Theoretical Intermediate Result (ng)} = \frac{(\text{Expected Result})}{(\text{Dilution Factor})}$$

where,

Expected Result	=	Expected Result from EQ. 1a (ng).
Dilution Factor	=	Reported Analysis/DilutionFactor. Default to 1 for deuterated monitoring compounds.

EQ. 8c Amount Found

$$\text{Amount found} = \frac{(\text{Response} \times \text{IS Expected Result})}{(\text{IS Response} \times \overline{\text{RRF}})}$$

where,

Amount found	=	Peak/IntermediateResult (ng).
Response	=	Reported Peak/Response.
IS Expected Result	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
IS Response	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
$\overline{\text{RRF}}$	=	Mean RRF from Equation 2a.

EQ. 9 Matrix Spike Recovery Calculation

$$\text{Matrix Spike Recovery} = \frac{\text{SSR} - \text{SR}}{\text{SA}} \times 100$$

where,

Matrix Spike Recovery	=	Analyte/PercentRecovery.
SSR	=	The Concentration value from EQ. 6 from the spike sample (µg/L).

SR = The Concentration value from EQ. 6 from the original sample (µg/L).

SA = Expected Concentration from EQ. 9a (µg/L).

EQ. 9a Expected Concentration

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

where,

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

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

Amount Added = Reported Analyte/AmountAdded (µL).

Injection Volume = Reported Analysis/InjectionVolume (mL).

EQ. 10 Relative Percent Difference Calculation

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

where,

RPD = Analyte/RPD

MSR = Matrix Spike Recovery from EQ. 9 from the MS sample.

MSDR = Matrix Spike Recovery from EQ. 9 from the MSD sample.

Equations for Exhibit D Low/Medium Volatiles

EQ. 1 Relative Response Factor Calculation

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

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 Percent Relative Standard Deviation Calculation

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

where,

%RSD	=	Peak/PercentRSD under the AnalysisGroup node.
SD_{RRF}	=	Standard Deviation from EQ. 3.
$\overline{X}$	=	Mean RRF from EQ. 4.

EQ. 3 Standard Deviation Calculation

$$\text{Standard Deviation} = \sqrt{\frac{\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}{(n-1)}}$$

where,

x_i = Relative Response Factor from EQ. 1 where the reported Peak/RRF is not null.

$\bar{x}$ = Mean Relative Response Factor from EQ. 4 where the reported Peak/RRF is not null.

n = Number of non-missing Relative Response Factor values.

EQ. 4 Mean Value Calculation

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

where,

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

X_i = Relative Response Factor EQ. 1 where the reported Peak/RRF is not null.

n = Number of non-missing Relative Response Factor values.

EQ. 5 Relative Response Factor Percent Difference Calculation

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

where,

$\%\text{Difference}_{RRF}$ = Peak/PercentDifference.

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

$\overline{RRF_i}$ = Mean Relative Response Factor from EQ. 4.

EQ. 6 Percent Moisture

$$\%\text{Moisture} = \frac{\text{grams of wet sample} - \text{grams of dry sample}}{\text{grams of wet sample}} \times 100$$

This equation is not calculated from the EDD.

EQ. 7 Water Concentration Calculation

$$\text{Concentration}\,(\mu g/L) = \left(\frac{A_x \times I_s}{A_{is} \times \overline{RRF}}\right)\left(\frac{DF}{V_o}\right)$$

where,

Concentration	=	Analyte/Result (µg/L).
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
I_s	=	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. 4.
DF	=	Reported Analysis/DilutionFactor. Default to 1 for deuterated monitoring compounds.
V_o	=	Reported Analysis/InjectionVolume (mL).

EQ. 8 Low-Level Soil/Sediment Concentration Calculation

$$\text{Concentration}\,(\mu g/Kg) = \left(\frac{A_x \times I_s}{A_{is} \times \overline{RRF}}\right)\left(\frac{DF}{W_s \times D}\right)$$

where,

Concentration	=	Analyte/Result (µg/kg).
A_x	=	Reported Peak/Response.
A_{is}	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
I_s	=	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. 4.
DF	=	Reported Analysis/DilutionFactor. Default to 1 for deuterated monitoring compounds.
W_s	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
D	=	Moisture Factor from EQ. 8a.

EQ. 8a Moisture Factor

$$\text{Moisture Factor} = \frac{(100 - \text{Percent Moisture})}{100}$$

where,

Percent Moisture = Reported SamplePlusMethod/PercentMoisture.

EQ. 9 Medium-Level Soil/Sediment Concentration Calculation

$$\text{Concentration}\,(\mu g/Kg) = \left(\frac{A_x \times I_s}{A_{is} \times \overline{RRF}}\right)\left(\frac{AV_t}{V_a}\right)\left(\frac{DF}{W_s \times D}\right)$$

where,

Concentration = Analyte/Result (µg/kg).

A_x = Reported Peak/Response.

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

I_s = 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. 4.

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).

D = Moisture Factor from EQ. 8a.

Note: EQ. 9 in the SOM01.1 SOW contains a value of 1000 in the numerator. This value converts the units of the term AV_t from mL to µL. EXES does not require this conversion factor because the term AV_t is calculated in units of µL from EQ. 9a.

EQ. 9a Adjusted Total Volume

$$AV_t = V_t + \left(\left(W_s - \left(W_s \times D\right)\right) \times 1000\right)$$

where,

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

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

D = Moisture Factor from EQ. 8a.

EQ. 10 Water Adjusted CRQL Calculation

$$\text{Adjusted CRQL} = (\text{Contract CRQL})\left(\frac{V_x}{V_o}\right)(\text{DF})$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	The CRQL value reported in Exhibit C – Volatiles (µg/L).
V_x	=	Contract sample volume (5.0 mL).
V_o	=	Reported Analysis/InjectionVolume (mL).
DF	=	Reported Analysis/DilutionFactor.

EQ. 11 Low-Level Soil Adjusted CRQL Calculation

$$\text{Adjusted CRQL} = (\text{Contract CRQL})\left(\frac{W_x}{W_s \times D}\right)$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	The CRQL value reported in Exhibit C – Volatiles (µg/kg)).
W_x	=	Contract sample weight (5.0 g).
W_s	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
D	=	Moisture Factor from EQ. 8a.

EQ. 12 Medium-Level Soil Adjusted CRQL Calculation

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

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	The CRQL value reported in Exhibit C – Volatiles (µg/kg).
W_x	=	Contract Sample weight (5.0 g).
W_s	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
D	=	Moisture Factor from EQ. 8a.
AV_t	=	Adjusted Total Volume from EQ. 9a (µL).
V_c	=	Contract soil methanol extract volume (5000 µL).
V_y	=	Contract soil aliquot volume (100 µL).

V_a = Reported Analysis/AnalyzedAmount (µL).

DF = Reported Analysis/DilutionFactor.

Note: EQ. 12 in the SOM01.1 SOW contains a value of 1000 in the numerator. This value converts the units of the term V_t from mL to µL. EXES does not require this conversion factor because the term V_t is already in units of µL.

EQ. 13 DMC Percent Recovery Calculation

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

where,

%R = Analyte/PercentRecovery.

Q_d = Intermediate Result from EQ. 13a (ng).

Q_a = Theoretical Intermediate Result from EQ. 13b (ng).

Note: EQ. 13 in the SOM01.1 SOW contains the term DF (Dilution Factor) in the numerator. EXES does not use this value because dilution factor is accounted for in the term Qa (Theoretical Intermediate Result) in EQ. 13b.

EQ. 13a Intermediate Result

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

where,

Intermediate Result = Analyte/IntermediateResult (ng).

Amount Found = Amount Found from EQ 13c (ng).

n = Number of non-missing Amount Found values.

EQ. 13b Theoretical Intermediate Result

$$\text{Theoretical Intermediate Result (ng)} = \frac{(\text{Expected Result} \times \text{Analyzed Amount})}{(\text{Dilution Factor})}$$

where,

Expected Result = Expected Result from EQ. 1a (ng).

Analyzed Amount = Reported Analysis/AnalyzedAmount (µL).

Dilution Factor = Reported Analysis/DilutionFactor. Default to 1 for deuterated monitoring compounds.

EQ. 13c Amount Found

$$\text{Amount found} = \frac{(\text{Response} \times \text{IS Expected Result})}{(\text{IS Response} \times \overline{\text{RRF}})}$$

where,

Amount found	=	Peak/IntermediateResult (ng).
Response	=	Reported Peak/Response.
IS Expected Result	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).
IS Response	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
$\overline{\text{RRF}}$	=	Mean RRF from Equation 2a.

EQ. 14 Matrix Spike Recovery Calculation

$$\text{Matrix Spike Recovery} = \frac{\text{SSR} - \text{SR}}{\text{SA}} \times 100$$

where,

Matrix Spike Recovery	=	Analyte/PercentRecovery.
SSR	=	The Concentration value from EQ. 7 (for water samples), EQ. 8 (for low-level soil/sediment samples) or EQ. 9 (for medium-level soil/sediment samples) from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 7 (for water samples), EQ. 8 (for low-level soil/sediment samples) or EQ. 9 (for medium-level soil/sediment samples) from the original sample (µg/L or µg/kg).
SA	=	Expected Concentration from EQ. 14a (µg/L or µg/kg).

EQ. 14a Expected Concentration

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

where,

Expected Concentration	=	Analyte/ExpectedResult (µg/L or µg/kg).
Standard Concentration	=	Reported Analyte/StandardConcentration (µg/L).
Amount Added	=	Reported Analyte/AmountAdded (µL).
Sample Amount	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node for soil/sediment samples, or Analysis/InjectionVolume for water samples (g or mL).

Moisture Factor = Moisture Factor from EQ. 8a. Default to 1 for water samples.

EQ. 15 Relative Percent Difference Calculation

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

where,

RPD = Analyte/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 Calculation

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

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 Percent Relative Standard Deviation Calculation

$$\%RSD = \frac{\text{Standard Deviation}}{\overline{RRF}} \times 100$$

$$\text{Standard Deviation} = \sqrt{\frac{\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}{(n-1)}}$$

where,

%RSD	=	Peak/PercentRSD under the AnalysisGroup node.
$\overline{RRF}$	=	Mean RRF from EQ. 2a.
x_i	=	Relative Response Factor from EQ. 1 where the reported Peak/RRF is not null.
$\bar{x}$	=	Mean Relative Response Factor from EQ. 2a where the reported Peak/RRF is not null.
n	=	Number of non-missing Relative Response Factor values.

EQ. 2a Mean Relative Response Factor

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

where,

$\overline{RRF}$	=	Peak/MeanRRF under the AnalysisGroup node.
RRF	=	Relative Response Factor from EQ. 1 where the reported Peak/RRF is not null.
n	=	Number of non-missing Relative Response Factor values.

EQ. 3 Relative Response Factor Percent Difference Calculation

$$\%\text{Difference}_{RRF} = \frac{RRF_c - \overline{RRF_i}}{\overline{RRF_i}} \times 100$$

where,

$\%\text{Difference}_{RRF}$ = Peak/PercentDifference.

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

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

EQ. 4 Percent Moisture

$$\%\text{Moisture} = \frac{\text{grams of wet sample} - \text{grams of dry sample}}{\text{grams of wet sample}} \times 100$$

This equation is not calculated from the EDD.

EQ. 5 Concentration of Water Sample

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

where,

Concentration = Analyte/Result (µg/L).

A_x = Reported Peak/Response.

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

I_s = 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. 2a.

DF = Reported Analysis/DilutionFactor.

V_a = Reported Analysis/AnalyzedAmount (µL).

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

V_o = Reported PreparationPlusCleanup/AliquotAmount from the preparation node (mL).

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. 6 Concentration of Soil/Sediment Sample

$$\text{Concentration } \mu g/Kg = \left(\frac{A_x \times I_s}{A_{is} \times \overline{RRF}}\right)\left(\frac{DF}{V_a}\right)\left(\frac{V_t}{W_t \times D}\right)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \cdots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_N$$

where,

Concentration = Analyte/Result (µg/kg).

A_x = Reported Peak/Response.

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

I_s = 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. 2a.

DF = Reported Analysis/DilutionFactor.

V_a = Reported Analysis/AnalyzedAmount (µL).

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

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

D = Moisture Factor from EQ. 6a.

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. 6a Moisture Factor

$$\text{Moisture Factor} = \frac{(100 - \text{Percent Moisture})}{100}$$

where,

Percent Moisture = Reported SamplePlusMethod/PercentMoisture.

EQ. 7 Aqueous Adjusted CRQL

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

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	The CRQL value reported in Exhibit C – Semivolatiles (µg/L).
V_x	=	Contract 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	=	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. 8 Soil/Sediment Adjusted CRQL

$$\text{Adjusted CRQL} = (\text{Contract CRQL})\left(\frac{W_x}{W_s \times D}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \ldots \left(\frac{CV_{out}}{CV_{in} \times E}\right)_N$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	The CRQL value reported in Exhibit C – Semivolatiles (µg/kg).
W_x	=	Contract sample weight (30 g for low-level soil/sediment samples and 1.0 g for medium-level soil/sediment samples).
W_s	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
D	=	Moisture Factor from EQ. 6a.
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. 9 DMC Percent Recovery Calculation

$$\text{Percent Recovery} = \frac{Q_d}{Q_a} \times 100$$

where,

Percent Recovery	=	Analyte/PercentRecovery.
Q_d	=	Intermediate Result from EQ. 9a (ng).
Q_a	=	Theoretical Intermediate Result from EQ. 9b (ng).

Note: EQ. 9 in the SOM01.1 SOW contains the term DF (Dilution Factor) in the numerator. EXES does not use this value because dilution factor is accounted for in the term Qa (Theoretical Intermediate Result) in EQ. 9b.

EQ. 9a Intermediate Result

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

where,

Intermediate Result	=	Analyte/IntermediateResult (ng).
Amount Found	=	Amount Found from EQ 9e (ng).
n	=	Number of non-missing Amount Found values.

EQ. 9b 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. 9c (ng).
Cleanup Factor	=	Cleanup Factor from EQ. 9d. Default to 1 if cleanup is not performed.

Injection Volume	=	Reported Analysis/InjectionVolume (µL).
Prep Final Amount	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL). Default to 1 for GPC Calibration Checks.
Dilution Factor	=	Reported Analysis/DilutionFactor.
Cleanup Initial Amount	=	Reported PreparationPlusCleanup/InitialAmount from the cleanup node for GPC Calibration Checks (µL). Default to 1 for all other analyses.

EQ. 9c 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. 9d 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. 9e Amount Found

$$\text{Amount found} = \frac{(\text{Response} \times \text{IS Expected Result} \times \text{Injection Volume})}{(\text{IS Response} \times \overline{\text{RRF}} \times \text{Analyzed Amount})}$$

where,

Amount found	=	Peak/IntermediateResult (ng).
Response	=	Reported Peak/Response.
IS Expected Result	=	Expected Result of the associated internal standard that is referenced in the PeakComparison node from EQ. 1a (ng).

Injection Volume	=	Reported Analysis/InjectionVolume (µL).
IS Response	=	Reported Peak/Response of the associated internal standard that is referenced in the PeakComparison node.
$\overline{RRF}$	=	Mean RRF from Equation 2a.
Analyzed Amount	=	Reported Analysis/AnalyzedAmount (µL).

EQ. 10 Matrix Spike Recovery Calculation

$$\text{Matrix Spike Recovery} = \frac{SSR - SR}{SA} \times 100$$

where,

Matrix Spike Recovery	=	Analyte/PercentRecovery.
SSR	=	The Concentration value from EQ. 5 (for water samples) or EQ. 6 (for soil/sediment samples) from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 5 (for water samples) or EQ. 6 (for soil/sediment samples) from the original sample (µg/L or µg/kg).
SA	=	Expected Concentration from EQ. 10a (µg/L or µg/kg).

EQ. 10a Expected Concentration

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

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).
Moisture Factor	=	Moisture Factor from EQ. 6a. Default to 1 for water samples.

EQ. 11 Relative Percent Difference Calculation

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

where,

RPD = Analyte/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 Pesticides

EQ. 1 Mean Absolute 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 for non-missing values where the Peak/CalibrationFactor is not null.

n = Number of non-missing RetentionTime values where the Peak/CalibrationFactor is not null.

EQ. 2 Calibration Factor

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

where,

CF = Peak/CalibrationFactor.

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

Mass Injected (ng) = Expected Intermediate Result from EQ. 2a (ng).

EQ. 2a Expected Intermediate Result

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

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 Peak/CalibrationFactor is not null.

n = Number of non-missing Calibration Factor values.

EQ. 4 Percent Relative Standard Deviation of the Calibration Factors

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

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

where,

%RSD = Peak/PercentRSD under the AnalysisGroup node.

SD_{CF} = Standard deviation of the Calibration Factors.

CF_i = Calibration Factor from EQ. 2 where the reported Peak/CalibrationFactor is not null.

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

n = Number of non-missing Calibration Factor values.

EQ. 5 Amount Found

$$\text{Amount found (ng)} = \frac{\text{Peak area (or Height) of compound}}{\overline{CF}}$$

where,

Amount found (ng) = Peak/IntermediateResult (ng).

Peak area (or Height) of compound = Reported Peak/Response.

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

EQ. 6 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. 5 (ng).
Amount (ng) of DDT injected	=	Expected Intermediate Result of DDT from EQ. 2a (ng).

EQ. 7 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 + endrin ketone)	=	Amount Found of endrin aldehyde + endrin ketone from EQ. 5 (ng).
Amount (ng) of Endrin injected	=	Expected Intermediate Result of Endrin from EQ. 2a (ng).

EQ. 8 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. 6.
%Breakdown	=	Percent Breakdown of Endrin from EQ. 7.

EQ. 9 Percent Difference Between the Calculated and Nominal Concentrations

$$\%\text{Difference} = \frac{\left(C_{calc} - C_{nom}\right)}{C_{nom}} \times 100$$

where,

%Difference	=	Peak/PercentDifference.
C_{calc}	=	Amount Found from EQ. 5 (ng).
C_{nom}	=	Expected Intermediate Result from EQ. 2a (ng).

EQ. 10 Percent Resolution

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

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

EQ. 11 **Percent Difference Between the Calibration Factor and the Mean Calibration Factor**

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

where,

%Difference	=	Peak/PercentDifference.
CF	=	Calibration Factor from EQ. 2.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 3.

EQ. 12 **Percent Moisture**

$$\%\text{Moisture} = \frac{\text{grams of wet sample} - \text{grams of dry sample}}{\text{grams of wet sample}} \times 100$$

This equation is not calculated from the EDD. This result is reported in the element SamplePlusMethod/PercentMoisture.

EQ. 13 **Percent Recovery**

$$\text{Percent Recovery} = \frac{Q_d}{Q_a} \times 100$$

where,

Percent Recovery	=	Analyte/PercentRecovery.
Q_d	=	Intermediate Result from EQ. 13a (ng).
Q_a	=	Theoretical Intermediate Result from EQ. 13b (ng).

Note: EQ. 13 in the SOM01.1 SOW contains the term DF (Dilution Factor) in the numerator. EXES does not use this value because dilution factor is accounted for in the term Qa (Theoretical Intermediate Result) in EQ. 13b.

EQ. 13a **Intermediate Result**

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

where,

Intermediate Result	=	Analyte/IntermediateResult (ng).
Amount Found	=	Amount Found from EQ 5 (ng).
n	=	Number of non-missing Amount Found values.

EQ. 13b Theoretical Intermediate Result

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

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 checks, and 1 for GPC Calibration Checks.
Dilution Factor	=	Reported Analysis/DilutionFactor.
Cleanup Initial Amount	=	Reported PreparationPlusCleanup/InitialAmount from the cleanup node for GPC Calibration Checks (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 Concentration Calculation of Target Compounds in Water Samples

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

where,

Concentration	=	Analyte/Result (µg/L). 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. 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 and 1000 for florisil cartridge checks.
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. 15 On-Column Concentration of Water Sample Extract

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

where,

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

EQ. 16 Concentration of Target Compounds in Soil/Sediment Samples

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

where,

Concentration	=	Analyte/Result (µg/kg). 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. 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).
D	=	Moisture Factor from EQ. 16a.
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. 16a Moisture Factor

$$\text{Moisture Factor} = \frac{(100 - \text{Percent Moisture})}{100}$$

where,

Percent Moisture	=	Reported SamplePlusMethod/PercentMoisture.

EQ. 17 On-Column Concentration of Soil Sample Extract

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

where,

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

EQ. 18 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 (for water samples) or EQ. 16 (for soil/sediment samples) from the two Analysis nodes where the analyte is detected on both GC columns (µg/L or µg/kg).
$Conc_H$	=	The lesser of the Concentration values from EQ. 14 (for water samples) or EQ. 16 (for soil/sediment samples) from the two Analysis nodes where the analyte is detected on both GC columns (µg/L or µg/kg).

EQ. 19 CRQL for Water Samples

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

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	The CRQL value reported in Exhibit C – Pesticides (µg/L).
V_x	=	Contract 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	=	Contract 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 CRQL for Soil/Sediment Samples

$$\text{Adjusted CRQL} = (\text{Contract CRQL})\left(\frac{W_x}{W_s \times D}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \ldots\left(\frac{CV_{out}}{CV_{in} \times E}\right)_N$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	The CRQL value reported in Exhibit C – Pesticides (µg/kg).
W_x	=	Contract sample weight (30 g).
W_s	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
D	=	Moisture Factor from EQ. 16a.
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).
V_y	=	Contract 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. 21 **Percent Recovery of Spike Compounds in MS/MSD Samples** (including LCS)

$$\text{Matrix Spike Recovery} = \frac{\text{SSR} - \text{SR}}{\text{SA}} \times 100$$

where,

Matrix Spike Recovery	=	Analyte/PercentRecovery.
SSR	=	The Concentration value from EQ. 14 (for water samples) or EQ. 16 (for soil/sediment samples) from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 14 (for water samples) or EQ. 16 (for soil/sediment samples) from the original sample (µg/L or µg/kg).
SA	=	Expected Concentration from EQ. 21a (µg/L or µg/kg).

EQ. 21a **Expected Concentration**

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

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).
Moisture Factor	=	Moisture Factor from EQ. 16a. Default to 1 for water samples.

EQ. 22 Relative Percent Difference Between MS/MSD Recoveries

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

where,

RPD	=	Analyte/RPD
MSR	=	Matrix Spike Recovery from EQ. 21 from the MS sample.
MSDR	=	Matrix Spike Recovery from EQ. 21 from the MSD sample.

Equations for Exhibit D Aroclors

EQ. 1 Mean Absolute 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 for non-missing values where the Peak/CalibrationFactor is not null.

n = Number of non-missing RetentionTime values where the Peak/CalibrationFactor is not null.

EQ. 2 Calibration Factor

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

where,

CF = Peak/CalibrationFactor.

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

Mass Injected (ng) = Expected Intermediate Result from EQ. 2a (ng).

EQ. 2a Expected Intermediate Result

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

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 Peak/CalibrationFactor is not null.
n	=	Number of non-missing Calibration Factor values.

EQ. 4 Percent Relative Standard Deviation of the Calibration Factors

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

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

where,

%RSD	=	Peak/PercentRSD under the AnalysisGroup node.
SD_{CF}	=	Standard deviation of the Calibration Factors.
CF_i	=	Calibration Factor from EQ. 2 where the reported Peak/CalibrationFactor is not null.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 3.
n	=	Number of non-missing Calibration Factor values.

EQ. 5 Percent Difference Between the Calibration Factor and the Mean Calibration Factor

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

where,

%Difference	=	Peak/PercentDifference.
CF	=	Calibration Factor from EQ. 2.
$\overline{CF}$	=	Mean Calibration Factor from EQ. 3.

EQ. 6 Percent Moisture

$$\%Moisture = \frac{\text{grams of wet sample} - \text{grams of dry sample}}{\text{grams of wet sample}} \times 100$$

This equation is not calculated from the EDD.

EQ. 7 Concentration Calculation for Water Samples

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

where,

Concentration	=	Analyte/Result (µg/L). 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 of Water Sample Extract

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

where,

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

EQ. 9 Concentration Calculation for Soil Samples

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

where,

Concentration	=	Analyte/Result (µg/kg). 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).
D	=	Moisture Factor from EQ. 9a.
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. 9a **Moisture Factor**

$$\text{Moisture Factor} = \frac{(100 - \text{Percent Moisture})}{100}$$

where,

Percent Moisture	=	Reported SamplePlusMethod/PercentMoisture.

EQ. 10 **On-Column Concentration of Soil Sample Extract**

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

where,

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

EQ. 11 **Percent Difference Calculation**

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

where,

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

EQ. 12 Adjusted CRQL Calculation for Water Samples

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

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/L).
Contract CRQL	=	The CRQL value reported in Exhibit C – Aroclors (µg/L).
V_x	=	Contract 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	=	Contract 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 Adjusted CRQL Calculation for Soil/Sediment Samples

$$\text{Adjusted CRQL} = (\text{Contract CRQL})\left(\frac{W_x}{W_s \times D}\right)\left(\frac{V_t}{V_y}\right)(DF)\left(\frac{CV_{out}}{CV_{in} \times E}\right)_1\left(\frac{CV_{out}}{CV_{in} \times E}\right)_2 \ldots\left(\frac{CV_{out}}{CV_{in} \times E}\right)_N$$

where,

Adjusted CRQL	=	ReportedResult/QuantitationLimit (µg/kg).
Contract CRQL	=	The CRQL value reported in Exhibit C – Aroclors (µg/kg).
W_x	=	Contract sample seight (30 g).
W_s	=	Reported PreparationPlusCleanup/AliquotAmount from the preparation node (g).
D	=	Moisture Factor from EQ. 9a.
V_t	=	Reported PreparationPlusCleanup/FinalAmount from the preparation node (µL).
V_y	=	Contract 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. 14 Surrogate Recovery Calculation

$$\text{Percent Recovery} = \frac{Q_d}{Q_a} \times 100$$

where,

Percent Recovery	=	Analyte/PercentRecovery.
Q_d	=	Intermediate Result from EQ. 14a (ng).
Q_a	=	Theoretical Intermediate Result from EQ. 14b (ng).

Note: EQ. 14 in the SOM01.1 SOW contains the term DF (Dilution Factor) in the numerator. EXES does not use this value because dilution factor is accounted for in the term Qa (Theoretical Intermediate Result) in EQ. 14b.

EQ. 14a Intermediate Result

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

where,

IntermediateResult	=	Analyte/IntermediateResult (ng).
Amount Found	=	Amount Found from EQ 14e (ng).
n	=	Number of non-missing Amount Found values.

EQ. 14b 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. 14c (ng).
Cleanup Factor	=	Cleanup Factor from EQ. 14d. 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 and 1 for GPC Calibration Checks.
Dilution Factor	=	Reported Analysis/DilutionFactor.
Cleanup Initial Amount	=	Reported PreparationPlusCleanup/InitialAmount from the cleanup node for GPC Calibration Checks (µL). Default to 1 for all other analyses.

EQ. 14c 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. 14d 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. 14e **Amount Found**

$$\text{Amount found} = \frac{\text{Peak area (or Height) of compound}}{\overline{\text{CF}}}$$

where,

Amount found	=	Peak/IntermediateResult (ng).
Peak area (or Height) of compound	=	Reported Peak/Response.
$\overline{\text{CF}}$	=	Mean Calibration Factor from EQ. 3.

EQ. 15 **Percent Recovery of Spike Compounds in MS/MSD Samples** (including LCS)

$$\text{Matrix Spike Recovery} = \frac{\text{SSR} - \text{SR}}{\text{SA}} \times 100$$

where,

Matrix Spike Recovery	=	Analyte/PercentRecovery.
SSR	=	The Concentration value from EQ. 7 (for water samples) or EQ. 9 (for soil/sediment samples) from the spike sample (µg/L or µg/kg).
SR	=	The Concentration value from EQ. 7 (for water samples) or EQ. 9 (for soil/sediment samples) from the original sample (µg/L or µg/kg).
SA	=	Expected Concentration from EQ. 15a (µg/L or µg/kg).

EQ. 15a **Expected Concentration**

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

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).
Moisture Factor	=	Moisture Factor from EQ. 9a. Default to 1 for water samples.

EQ. 16 Relative Percent Difference Between MS/MSD Recoveries

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

where,

RPD	=	Analyte/RPD
MSR	=	Matrix Spike Recovery from EQ. 15 from the MS sample.
MSDR	=	Matrix Spike Recovery from EQ. 15 from the MSD sample.

Figure 1: SEDD Data Node Hierarchy