APPENDIX D

Data Management

Appendix D   Data Management Rules

D.1   LABORATORY REPLICATE SAMPLES

Chemical concentrations obtained from the analysis of laboratory duplicate or replicate samples (two or more analyses on the same sample) are averaged for a closer representation of the "true" concentration as compared to the results of a single analysis. Averaging rules are dependent on whether the individual results are detected concentrations or reporting limits (RLs) for undetected analytes. If all concentrations are detects for a given parameter, the values are simply averaged arithmetically. If all concentrations are undetected for a given parameter, the minimum RL is reported. If the concentrations are a mixture of detected concentrations and RLs, any two or more detected concentrations are averaged arithmetically and RLs are ignored. If there is a single detected concentration and one or more RLs, the detected concentration is reported. The latter two rules are applied regardless of whether the RLs are higher or lower than the detected concentration.

D.2   LOCATION AVERAGING

Chemical concentrations for a single location where more than one sample is obtained are calculated as the average concentration of a surface sediment sample and the associated field duplicate sample. These types of samples are also called field splits (PSEP 1997), and are collected at a single location using the same homogenized sediment. The sample and the field duplicate sample are submitted to the laboratory as individual samples, and they are analyzed separately. The averaging rules used for location averaging are the same as for laboratory replicate samples described above. A sampling location with averaged chemical concentrations is presented as a single "sample" in the data report text and data tables.

D.3   SIGNIFICANT FIGURES AND ROUNDING

The laboratories report results with different numbers of significant figures depending on the instrument, parameter, and the concentration relative to the reporting limit (RL). The reported (or assessed) precision of each observation is explicitly stored in the project database as a record of the number of significant figures assigned by the laboratory. The tracking of significant figures becomes important when calculating averages and performing other data summaries.

When a calculation involves addition, such as totaling polychlorinated biphenyls (PCBs) or polycyclic aromatic hydrocarbons (PAHs), the calculation can only be as precise as the least precise number that went into the calculation. For example (assuming two significant figures):

> 210 + 19 = 229, but this would be reported as 230 because the trailing zero in the number 210 is not significant.

When a calculation involves multiplication or division, such as when organic carbon normalizing is used, all significant figures are carried through the calculation, and then the total result is rounded at the end of the calculation to reflect the value used in the calculation with the fewest significant figures. For example:

59.9 x 1.2 = 71.88, to be reported as 72 because there are two significant figures in the number 1.2.

When rounding, if the number following the last significant figure is less than 5, the digit is left unchanged. If the number following the last significant figure is equal to or greater than 5, the digit is increased by 1.

Many of the Washington State Sediment Management Standards (SMS) chemical criteria are in units normalized to the total organic carbon (TOC) content in the sediment sample (mg/kg OC). Only samples with TOC concentrations ≥0.5% or ≤4.0% are considered appropriate for organic carbon normalization. Samples with TOC concentrations <0.5% or >4.0% are compared to dry weight chemical criteria. Chemical concentrations originally in units of μg/kg dry weight were converted to mg/kg OC using the following equation:

$$\frac{(C_{\mu g/kg\ dry\ weight}) \times (0.001\ mg/\mu g)}{TOC}$$

Where:

C = the chemical concentration
TOC = the percent total organic carbon on a dry weight basis, expressed as a decimal (e.g., 1% = 0.01)]

D.4   DILUTIONS

All analyte concentrations within the calibration range of the instrument in the lowest analytical dilution are selected as the final result. Any analyte concentrations that exceed the calibration range and are qualified as estimated by the laboratory as an exceedance (E-qualified) are rejected by the data validator. The values for these analytes are selected from the analysis of the sample dilution in which the analyte concentration is within the calibration range of the instrument. In cases where the result from the lowest analytical dilution is qualified by the laboratory or the validator, the validator uses best professional judgment to determine whether or not the qualification warrants the selection of the result from another analytical dilution as the final result.

D.5   MULTIPLE RESULTS FOR THE SAME ANALYTE USING ONE ANALYTICAL METHOD

Multiple analyses of a sample for a group of analytes can occur as a result of laboratory quality assurance (QA) issues that may only affect a subset of the analyte group. In these cases, there may be multiple results for certain analytes. The data

validator uses the following rules to select a single value when multiple results are reported by the laboratory for a single analyte in a single sample using the same method.

- If all results are detected without qualification as an estimated value (i.e., J- or E-qualifier), then the result from the lowest analytical dilution is selected. If multiple, unqualified results from the same analytical dilution are available the highest concentration is selected as a health-protective approach.

- If a mixture of estimated (i.e., J-qualified) and unqualified detected results are reported, then the unqualified detected result is selected.

- If all results are reported as detected with estimated qualification, the "best result" is selected using best professional, technical judgment.

- If both undetected and detected results are reported, then the detected result is selected.

- If all results are reported as undetected, then the lowest RL is selected.

D.6 MULTIPLE RESULTS FOR AN ANALYTE DETERMINED BY DIFFERENT ANALYTICAL METHODS

In cases where a single analyte is reported by more than one method, the preferred method is identified in the quality assurance project plan (QAPP). The results of this method are selected as the final value by the data validator unless the validator identifies a QA issue that warrants the selection of the results from an alternative method. These instances and the justification for decisions are documented in the data validation report. In cases where the results are generated in two separate analytical groups that are not submitted to the validator together, the QA manager is responsible for evaluating the results and determining the most appropriate final result.

D.7 CALCULATING TOTALS

Concentrations for analyte sums are calculated as follows:

- **Total PCBs** are calculated, in accordance with the methods of the Washington State Sediment Management Standards (SMS), using only detected values for seven Aroclor mixtures.[1] For individual samples in which none of the seven Aroclor mixtures is detected, total PCBs are given a value equal to the highest RL of the seven Aroclors and assigned a U-qualifier indicating the lack of detected concentrations.

- **Total low-molecular-weight PAHs (LPAHs), high-molecular-weight PAHs (HPAHs), PAHs, and benzofluoranthenes** are also calculated in accordance with the methods of the SMS. Total LPAHs are the sum of detected concentrations for naphthalene, acenaphthylene, acenaphthene, fluorene,

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[1] Aroclors 1016, 1221, 1232, 1242, 1248, 1254, and 1260.

phenanthrene, and anthracene. Total HPAHs are the sum of detected concentrations for fluoranthene, pyrene, benzo(a)anthracene, chrysene, total benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3,-c,d)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene. Total benzofluoranthenes are the sum of the b (i.e., benzo(b)fluoranthene), j, and k isomers. Because the j isomer is rarely quantified, this sum is typically calculated with only the b and k isomers. For samples in which all individual compounds within any of the three groups described above are undetected, the single highest RL for that sample represents the sum.

◆ **Total DDTs** are calculated using only detected values for the six DDT isomers: 2,4'-DDD; 4,4'-DDD; 2,4'-DDE; 4,4'-DDE; 2,4'-DDT; and 4,4'-DDT. For individual samples in which none of the isomers are detected, total DDTs are given a value equal to the highest RL of the six isomers and assigned a U-qualifier, indicating the lack of detected concentrations.

◆ **Total chlordane** is calculated using only detected values for the following compounds: alpha-chlordane, gamma-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor. For individual samples in which none of these compounds is detected, total chlordane is given a value equal to the highest RL of the five compounds listed above and assigned a U-qualifier, indicating the lack of detected concentrations.

◆ **Total petroleum hydrocarbon (TPH)** is calculated as the sum of the detected concentrations of the diesel and oil fractions. For individual samples in which neither diesel nor oil is detected, TPH is given a value equal to the highest RL of the individual fractions and assigned a U-qualifier indicating the lack of detected concentrations. Results generated using the Northwest total petroleum hydrocarbon – hydrocarbon identification (NWTPH-HCID) or Northwest total petroleum hydrocarbon – gasoline (NWTPH-G) methods are not calculated in this total.

D.8 CALCULATION OF PCB CONGENER TEQS

PCB congener toxic equivalents (TEQs) are calculated using the World Health Organization (WHO) consensus toxic equivalency factor (TEF) values (Van den Berg et al. 2006) for mammals as presented in Table D-1. The TEQ is calculated as the sum of each congener concentration multiplied by the corresponding TEF value. When the congener concentration is reported as non-detected, then the TEF is multiplied by zero, half the RL or the full RL, depending on the calculation method specified.

Table D-1. PCB congener TEF values for mammals

PCB Congener Number	TEF Value (unitless)
77	0.0001
81	0.0003
105	0.00003
114	0.00003
118	0.00003
123	0.00003
126	0.1
156	0.00003
157	0.00003
167	0.00003
169	0.03
189	0.00003

D.9 CALCULATION OF DIOXIN/FURAN CONGENER TEQS

Dioxin/furan congener TEQs are calculated using the WHO consensus TEF values (Van den Berg et al. 2006) for mammals as presented in Table E-2. The TEQ is calculated as the sum of each congener concentration multiplied by the corresponding TEF value. When the congener concentration is reported as undetected, then the TEF is multiplied by zero, half the RL, or the full RL, depending on the calculation method specified.

Table D-2. Dioxin/furan congener TEF values for mammals

Dioxin/Furan Congener	TEF Value (unitless)
1,2,3,4,6,7,8-Heptachlorodibenzofuran	0.01
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	0.01
1,2,3,4,7,8,9-Heptachlorodibenzofuran	0.01
1,2,3,4,7,8-Hexachlorodibenzofuran	0.1
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	0.1
1,2,3,6,7,8-Hexachlorodibenzofuran	0.1
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	0.1
1,2,3,7,8,9-Hexachlorodibenzofuran	0.1
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	0.1
1,2,3,7,8-Pentachlorodibenzofuran	0.03
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	1
2,3,4,6,7,8-Hexachlorodibenzofuran	0.1
2,3,4,7,8-Pentachlorodibenzofuran	0.3
2,3,7,8-Tetrachlorodibenzofuran	0.1
2,3,7,8-Tetrachlorodibenzo-p-dioxin	1
Octachlorodibenzofuran	0.0003
Octachlorodibenzo-p-dioxin	0.0003

D.10 CALCULATION OF CARCINOGENIC POLYCYCLIC AROMATIC HYDROCARBONS

Carcinogenic polycyclic aromatic hydrocarbons (cPAH) values were calculated using TEF values (California EPA 1994; Ecology 2001) based on the individual PAH component's relative toxicity to benzo(a)pyrene. TEF values are presented in Table E-3. The cPAH was calculated as the sum of each individual PAH concentration multiplied by the corresponding TEF value. When the individual PAH component concentration was reported as non-detected, then the TEF was multiplied by half the RL.

Table D-3. cPAH TEF values

cPAH	TEF Value (unitless)
Benzo(a)pyrene	1
Benzo(a)anthracene	0.1
Benzo(b)fluoranthene	0.1
Benzo(k)fluoranthene	0.1
Dibenz(a,h)anthracene	0.4
Indeno(1,2,3-cd)pyrene	0.1
Chrysene	0.01

cPAH – carcinogenic polycyclic aromatic hydrocarbon

TEF – toxic equivalency factor

D.11 DATA QUALITY

Data used in the T-117 Engineering Evaluation/Cost Assessment (EE/CA) must be relevant and of sufficient data quality. Data may be excluded from the T-117 EE/CA for the following reasons:

◆ If the sample has been removed from the site after the sample was collected (e.g., upland soil that has been excavated, and sediment samples that have been dredged)

◆ If data quality is determined to be insufficient (e.g., the data have not been validated and/or supportive documentation is not available so the accuracy of the data can not be verified)

◆ If the data are too old to be considered reflective of current site conditions (i.e., the samples were collected prior to 1990)

E.12 REFERENCES

PSEP. 1997. Recommended guidelines for sampling marine sediment, water column, and tissue in Puget Sound. Final report. Prepared for the US Environmental Protection Agency, Seattle, WA. Puget Sound Water Quality Action Team, Olympia, WA.

Van den Berg M, Birnbaum LS, Denison M, De Vito M, Farland W, Feeley M, Fiedler H, Hakansson H, Hanberg A, Haws L, Rose M, Safe S, Schrenk D, Tohyama C, Tritscher A, Tuomisto J, Tysklind M, Walker N, Peterson RE. 2006. The 2005 World Health Organization reevaluation of human and mammalian toxic equivalency factors for dioxins and dioxin-like compounds. Tox Sci 93(2):223-241.