Attachment 3 Data Management Rules

LABORATORY REPLICATES

Chemical concentrations obtained from the analysis of laboratory duplicates or replicates (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.

LOCATION AVERAGING

The baseline surface sediment dataset contains averaged results of chemical concentrations of discrete samples collected at a single sampling location that were submitted to the laboratory as individual samples and analyzed separately. The averaging rules used for location averaging are the same as for laboratory replicates described above. A sampling location with averaged chemical concentrations is presented as a single "sample" in the ERA text and data tables. This type of averaging is performed in the following instances.

- The chemical concentrations obtained from the analyses of a surface sediment sample, and its field duplicate or replicate, are averaged to obtain a single concentration of the chemical for the sampling location.
- Surface sediment data have been collected repeatedly at certain locations within a six-month period.[1] For these locations that have multiple samples collected at different times, the results of these individual samples are averaged to a single chemical concentration for that location.

[1] An assumption was made in the memorandum describing the baseline surface sediment dataset (Windward 2006) that two or more samples collected from the same location within a six-month period reflect spatial variability, rather than temporal variability. Therefore, these results were averaged together. For multiple samples collected more than six months apart from the same location, such as data collected within monitoring programs, any differences in chemical concentrations also reflect temporal variability. Therefore, only the most recent sample from those locations was included in the baseline surface sediment dataset; no averaging occurred in these situations.

- The baseline surface sediment dataset contains two locations that were re-sampled in a different sampling event, outside of a monitoring program. These sample results were also averaged to obtain a single representative result for that location.

SIGNIFICANT FIGURES AND ROUNDING

The laboratories reported 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 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.

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.

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.

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.

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.[2] 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.

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

- **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, 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.

CALCULATION OF PCB CONGENER TEQS

PCB congener toxic equivalents (TEQs) are calculated using the World Health Organization (WHO) consensus toxic equivalency factor (TEF) values for fish, birds (Van den Berg et al. 1998) and mammals (Van den Berg et al. 2006) as presented in Table 3-1. 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 1. PCB congener TEF values

PCB CONGENER NUMBER	TEF VALUE FOR FISH (unitless)	TEF VALUE FOR BIRDS (unitless)	TEF VALUE FOR MAMMALS (unitless)
77	0.0001	0.05	0.0001
81	0.0005	0.1	0.0003
105	<0.000005	0.0001	0.00003
114	<0.000005	0.0001	0.00003
118	<0.000005	0.00001	0.00003

PCB Congener Number	TEF Value for Fish (unitless)	TEF Value for Birds (unitless)	TEF Value for Mammals (unitless)
123	<0.000005	0.00001	0.00003
126	0.005	0.1	0.1
156	<0.000005	0.0001	0.00003
157	<0.000005	0.0001	0.00003
167	<0.000005	0.00001	0.00003
169	0.00005	0.001	0.03
189	<0.000005	0.00001	0.00003

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