APPENDIX A. DATA MANAGEMENT RULES

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Tables

Acronyms

cPAH	carcinogenic polycyclic aromatic hydrocarbon
DDD	dichlorodiphenyldichloroethane
DDE	dichlorodiphenyldichloroethylene
DDT	dichlorodiphenyltrichloroethane
EPA	US Environmental Protection Agency
HPAH	high-molecular-weight polycyclic aromatic hydrocarbon
HpCDD	heptachlorodibenzo-p-dioxin
HpCDF	heptachlorodibenzofuran
HxCDD	hexachlorodibenzo-p-dioxin
HxCDF	hexachlorodibenzofuran
LPAH	low-molecular-weight polycyclic aromatic hydrocarbon
PAH	polycyclic aromatic hydrocarbon
PCB	polychlorinated biphenyl
PeCDD	pentachlorodibenzo-*p*-dioxin
PeCDF	pentachlorodibenzofuran
PEF	potency equivalency factor
QC	quality control
RI/FS	remedial investigation and feasibility study
RL	reporting limit
SIM	selected ion monitoring
SMS	Washington State Sediment Management Standards
SVOC	semivolatile organic compound
TCDD	tetrachlorodibenzo-*p*-dioxin
TCDF	tetrachlorodibenzofuran
TEF	toxic equivalency factor
TEQ	toxic equivalent
WHO	World Health Organization

A.1 Data Management Rules

Data management rules being followed for this data compilation are the same as those applied to the remedial investigation/feasibility study (RI/FS) dataset, except as noted in this section. Rules summarized in this appendix include those used for averaging duplicate or replicate samples (Section A.1), selecting the preferred result if more than one result was reported for a chemical (Section A.2), handling significant figures and rounding (Section A.3), calculating totals when results are summed for individual components (Section A.4), calculating toxic equivalents (TEQs) for polychlorinated biphenyl (PCB) congeners and dioxin/furan congeners (Sections A.5 and A.6), and calculating carcinogenic polycyclic aromatic hydrocarbons (cPAHs) (Section A.7). Final data rules are provided in Appendix C of the Pre-Design Studies Work Plan (Windward and Integral [in prep]).

A.1.1 Averaging Laboratory Duplicate or Replicate Samples

Contaminant concentrations obtained from the analysis of laboratory duplicates or replicates (i.e., two or more analyses on the same sample) were averaged for a closer representation of the "true" concentration than that provided by the results of a single analysis. Averaging rules were dependent on whether the individual results were detected concentrations or reporting limits (RLs) for non-detected analytes. If all concentrations were detected for a given parameter, the values were simply averaged arithmetically. If all concentrations were non-detected for a given parameter, the minimum RL was reported. If the concentrations were a mixture of detected concentrations and RLs, any two or more detected concentrations were averaged arithmetically, and RLs were ignored. If there was one detected concentration and one or more RLs, the detected concentration was reported. The latter two rules were applied regardless of whether the RLs were higher or lower than the detected concentration.

A.1.2 Selection of Preferred Results

In some instances, the laboratory generated more than one result for a chemical for a given sample. Multiple results occurred for several reasons, including:

- The original result did not meet the laboratory's internal quality control (QC) guidelines, and a reanalysis was performed.
- The original result did not meet other project data quality objectives, such as a sufficiently low RL, and a reanalysis was performed.
- Two different analytical methods were used for that chemical.

In each case, a single result was selected for use. The procedures for selecting the preferred result differed depending on whether a single or multiple analytical methods were used for that chemical.

For the same analytical method, the results were selected using the following guidance:

- If the results were detected and not qualified, then the result from the lowest dilution was selected, unless multiple results from the same dilution were available, in which case the result with the highest concentration was selected.
- If the results were combination of estimated and unqualified detected results, then the unqualified result was selected. This situation most commonly occurred when the original result was outside of the calibration range, thus requiring a dilution. The diluted result within the calibration range was preferentially selected.
- If the results were all estimated, then the result was selected using best professional judgment and considering the rationale for qualification. For example, a result qualified based on laboratory replicate results outside of QC objectives for precision was preferred to a qualified result that was outside the calibration range.
- If the results were a combination of detected and non-detected results, then the detected result was selected. If there were more than one detected result, the applicable rules for multiple results (as discussed above) were followed.
- If the results were all non-detected, then the lowest RL was selected.

For different analytical methods (i.e., when a specific chemical was analyzed in the same sample using different methods), the following rules were applied:

- For results analyzed using the semivolatile organic compound (SVOC) full-scan (EPA 8270) and selected ion monitoring (SIM) (EPA 8270-SIM) methods, the SIM results were selected.
- For results analyzed using US Environmental Protection Agency (EPA) Method 8081A and any 8270 method (i.e., hexachlorobenzene and hexachlorocyclopentadiene), the 8081A result were selected.

The RI/FS database rules for the selection of preferred results between two methods (as described above) were revised for the compilation of the pre-design data. In the RI/FS, the preferred result was selected based on a comparison among the methods of the detection status, RL, and data qualifiers. The revised rules selected the preferred result based on a preference for method.

A.1.3 SIGNIFICANT FIGURES AND ROUNDING

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

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

> 210 + 19 = 229 was reported as 230 because 19 was only reported to 2 significant digits, and the enhanced precision of the trailing 0 in the number 210 was not significant.

When a calculation involved multiplication or division, such as carbon normalization, the original figures for each value were carried through the calculation (i.e., individual values were not adjusted to a standard number of significant figures; instead, the appropriate adjustment was made to the resultant value at the end of the calculation). The result was rounded at the end of the calculation to reflect the value with the fewest significant figures used in the calculation. For example:

> 59.9 x 1.2 = 71.88 was reported as 72 because there were 2 significant figures in the number 1.2.

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

A.1.4 CALCULATING TOTALS

Total PCBs, total dichlorodiphenyltrichloroethanes (DDTs), total PAHs, total chlordane, total xylenes, and total nitrosamines were calculated by summing the detected values for the individual components (e.g., Aroclor mixtures or individual congeners for total PCBs). For samples in which none of the individual components were detected, the total value was given as the highest RL of any individual component, and assigned a U-qualifier (no detected concentrations). No sum was calculated in cases where 50% or less of the components were analyzed. Concentrations for analyte sums were calculated using the following components:

- Total PCBs were calculated, in accordance with the methods of the Washington State Sediment Management Standards (SMS), using only detected values for all Aroclor mixtures. For individual samples in which none of the Aroclor mixtures were detected, total PCBs were given a value equal to the highest RL of the Aroclors and assigned a U-qualifier (no detected concentrations).

- Total low-molecular-weight PAHs (LPAHs), high-molecular-weight PAHs (HPAHs), PAHs, and benzofluoranthenes were also calculated in accordance with the methods of the SMS. Total LPAHs were the sum of detected concentrations for naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, and anthracene. Total HPAHs were 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 were the sum of the b (i.e., benzo(b)fluoranthene), j, and k isomers.

  Because the j isomer is rarely quantified, the total benzofluoranthenes sum was typically calculated with only the b and k isomers. In cases where the laboratory provided total benzofluoranthenes instead of or in addition to the b and k isomers, the laboratory result was reported, and no sum was calculated. For samples in which all individual compounds within any of the three groups described above were non-detected, the highest RL for that sample represented the sum.

- Total DDTs were calculated using only detected values for the DDT isomers: 2,4′-dichlorodiphenyldichloroethane (DDD); 4,4′-DDD; 2,4′-dichlorodiphenyldichloroethylene (DDE); 4,4′-DDE; 2,4′-DDT; and 4,4′-DDT. For individual samples in which none of the isomers were detected, total DDTs were given a value equal to the highest RL of the six isomers and assigned a U-qualifier (no detected concentrations).

- Total chlordane was 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 were detected, total chlordane was given a value equal to the highest RL of the five compounds listed and assigned a U-qualifier (no detected concentrations).

- Total xylene was calculated using only detected values for m,p-xylene and o-xylene. For individual samples in which neither of these compounds were detected, total xylene was given a value equal to the higher RL of the two compounds listed and assigned a U-qualifier (no detected concentrations).

- Total nitrosamines were calculated using only detected values for n-nitrodiethylamine, n-nitrosodimethylamine, n-nitroso-di-n-butylamine, n-nitroso-di-n-propylamine, and n-nitrosodiphenylamine. For individual samples in which none of these compounds were detected, total nitrosamines were given a value equal to the highest RL of the five compounds listed and assigned a U-qualifier (no detected concentrations).

A.1.5 CALCULATION OF PCB CONGENER TOXIC EQUIVALENTS

PCB congener TEQs were calculated using the World Health Organization (WHO) consensus toxic equivalency factor (TEF) values for mammals (Van den Berg et al. 1998; Van den Berg et al. 2006), as presented in Table 1. The TEQ was calculated as the sum of each PCB congener concentration multiplied by the corresponding TEF value. When the PCB congener concentration was reported as non-detected, then the TEF was multiplied by one-half the RL.

Table A-1. PCB congener TEF values

PCB Congener No.	TEF Value for Mammals (unitless)[a]
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

[a] From Van den Berg et al. (2006).
PCB – polychlorinated biphenyl
TEF – toxic equivalency factor

A.1.6 CALCULATION OF DIOXIN/FURAN CONGENER TEQS

Dioxin / furan congener TEQs were calculated using the WHO consensus TEF values for mammals (Van den Berg et al. 1998; Van den Berg et al. 2006), as presented in Table 2. The TEQ was calculated as the sum of each dioxin / furan congener concentration multiplied by the corresponding TEF value. When the dioxin / furan congener concentration was reported as non-detected, then the TEF was multiplied by one-half the RL.

Table A-2. Dioxin/furan congener TEF values

Dioxin/Furan Congener	TEF Value for Mammals (unitless)[a]
1,2,3,4,6,7,8-HpCDF	0.01
1,2,3,4,6,7,8-HpCDD	0.01
1,2,3,4,7,8,9-HpCDF	0.01

Dioxin/Furan Congener	TEF Value for Mammals (unitless)[a]
1,2,3,4,7,8-HxCDF	0.1
1,2,3,4,7,8-HxCDD	0.1
1,2,3,6,7,8-HxCDF	0.1
1,2,3,6,7,8-HxCDD	0.1
1,2,3,7,8,9-HxCDF	0.1
1,2,3,7,8,9-HxCDD	0.1
1,2,3,7,8-PeCDF	0.03
1,2,3,7,8-PeCDD	1
2,3,4,6,7,8-HxCDF	0.1
2,3,4,7,8-PeCDF	0.3
2,3,7,8-TCDF	0.1
2,3,7,8-TCDD	1
OCDF	0.0003
OCDD	0.0003

[a] From Van den Berg et al. (2006).

HpCDD – heptachlorodibenzo-*p*-dioxin
HpCDF – heptachlorodibenzofuran
HxCDD – hexachlorodibenzo-*p*-dioxin
HxCDF – hexachlorodibenzofuran
OCDD – octachlorodibenzo-*p*-dioxin
OCDF – octachlorodibenzofuran
PeCDD – pentachlorodibenzo-*p*-dioxin
PeCDF – pentachlorodibenzofuran
TCDD – tetrachlorodibenzo-*p*-dioxin
TCDF – tetrachlorodibenzofuran
TEF – toxic equivalency factor

A.1.7 Calculation of Carcinogenic Polycyclic Aromatic Hydrocarbons

cPAH values were calculated using potency equivalency factor (PEF) values (California EPA 2009) based on the individual PAH component's relative toxicity to benzo(a)pyrene. PEF values are presented in Table 3. The cPAH value was calculated as the sum of each individual PAH concentration multiplied by the corresponding PEF value. When the individual PAH component concentration was reported as non-detected, then the PEF was multiplied by one-half the RL.

Table A-3. cPAH PEF values

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

[a] PEFs for cPAHs are defined by California EPA (2009) by dividing the inhalation unit risk factor for the compound by the inhalation unit risk factor for benzo[a]pyrene.

cPAH – carcinogenic polycyclic aromatic hydrocarbon

EPA – US Environmental Protection Agency

PEF – potency equivalency factor

A.2 References

California EPA. 2009. Technical support document for cancer potency factors: methodologies for derivation, listing of available values, and adjustments to allow for early life stage exposures. Air Toxicology and Epidemiology Branch, Office of Environmental Health Hazard Assessment, California Environmental Protection Agency, Sacramento, CA.

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