

# APPENDIX C

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## Data Management



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### **AVERAGING LABORATORY REPLICATE SAMPLES**

Chemical concentrations obtained from the analysis of laboratory replicate samples (two or more analyses of the same sample) will be averaged for a closer representation of the “true” concentration as compared to the result of a single analysis. Averaging rules are dependent on whether the individual results are detected concentrations or reporting limits (RLs) for undetected chemicals. If all concentrations are detected for a single chemical, the values are simply averaged arithmetically for the sample and its associate laboratory replicate sample(s). If all concentrations are undetected for a given parameter, the minimum RL is selected. If the concentrations are a mixture of detected concentrations and RLs, any two or more detected concentrations are averaged arithmetically and RLs 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.

### **SIGNIFICANT FIGURES AND CALCULATIONS**

Analytical laboratories report results with various numbers of significant figures depending on the laboratory’s standard operating procedures, the instrument, the chemical, and the reported chemical concentration relative to the RL. The reported (or assessed) precision of each result is explicitly stored in the project database by recording the number of significant figures. Tracking of significant figures is used when calculating analyte sums and performing other data summaries. When a calculation involves addition, such as totaling PCBs, the calculation can only be as precise as the least precise number that went into the calculation. For example:

$210 + 19 = 229$  would be reported as 230 because although 19 is reported to 2 significant digits, the trailing zero in the number 210 is not significant.

When a calculation involves multiplication or division, the final result is rounded at the end of the calculation to reflect the value used in the calculation with the fewest significant figures. For example:

$59.9 \times 1.2 = 71.88$  would 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.

### **BEST RESULT SELECTION FOR MULTIPLE RESULTS**

In some instances, the laboratory generates more than one result for a chemical for a given sample. Multiple results can occur for several reasons, including: 1) the original

result did not meet the laboratory's internal quality control (QC) guidelines, and a reanalysis was performed; 2) the original result did not meet other project data quality objectives, such as a sufficiently low RL, and a reanalysis was performed; or 3) two different analytical methods were used for that chemical. In each case, a single best result is selected for use. The procedures for selecting the best result differ depending on whether a single or multiple analytical methods are used for that chemical.

For the same analytical method, if the results are:

- ◆ Detected and not qualified, then the result from the lowest dilution is selected, unless multiple results from the same dilution are available, in which case, the result with the highest concentration is selected.
- ◆ A combination of estimated and unqualified detected results, then the unqualified result is selected. This situation most commonly occurs when the original result is outside of calibration range, thus requiring a dilution.
- ◆ All estimated, then the "best result" is selected using best professional judgment in consideration of the rationale for qualification. For example, a result qualified based on laboratory replicate results outside of QC objectives for precision would be preferred to a qualified result that is outside the calibration range.
- ◆ A combination of detected and undetected results, then the detected result is selected. If there is more than one detected result, the applicable rules for multiple results (as discussed above) are followed.
- ◆ All undetected results, then the lowest RL is selected.

If the multiple results are from different analytical methods, then the result from the preferred method specified in the quality assurance project plan (QAPP) or based on the consensus of the professional opinions of project chemists was selected.

The following rules are applied to multiple results from different analytical methods:

- ◆ For detected concentrations analyzed by the SVOC full-scan and selective ion monitoring (SIM) methods (i.e., PAHs), the highest detected concentration is selected. If the result by one method is detected and the result by the other method is not detected, then the detected result is selected for reporting, regardless of the method. If results are reported as non-detected by both methods, the undetected result with the lowest RL is selected. The SIM method is more analytically sensitive than the full-scan SVOC method, and the undetected results are generally reported at a lower RL by the SIM method than by the full-scan method. Therefore, the SIM method is selected for non-detected results unless an analytical dilution or analytical interferences elevated the SIM RL above the SVOC full-scan RL.
- ◆ Hexachlorobenzene and hexachlorocyclopentadiene are analyzed by EPA Methods 8081A, 8270, and/or 8270-SIM. The result from the method with the

greatest sensitivity (i.e., lowest RL) is selected if all results are undetected. EPA Method 8081A results are generally selected, when available, because the standard laboratory RLs from this analysis are significantly lower than those from EPA Methods 8270 and 8270-SIM. When chemicals are detected, the detected result with the highest concentration is selected unless the detected concentration is qualified as estimated or tentatively identified, in which case the rule designating treatment of qualified and unqualified data would apply.

## CALCULATED TOTALS

Total PCBs, total dichloro-diphenyl-trichloroethane (DDTs), total PAHs, and total chlordane are calculated by summing the detected values for the individual components available for each sample. For individual samples in which none of the individual components is detected, the total value is given a value equal to the highest RL of an individual component, and assigned the same qualifier (U or UJ), indicating an undetected result. Concentrations for the analyte sums are calculated as follows:

- ◆ **Total PCBs** are calculated, in accordance with the methods of the SMS, using only detected values for seven Aroclor mixtures.<sup>1</sup> 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, 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 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.

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<sup>1</sup> Aroclors 1016, 1221, 1232, 1242, 1248, 1254, and 1260.

- ◆ **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 CARCINOGENIC POLYCYCLIC AROMATIC HYDROCARBONS

Carcinogenic polycyclic aromatic hydrocarbons (cPAH) values are calculated using potency equivalency factor (PEF) values (California EPA 2002; Ecology 2001) based on the individual PAH component's relative toxicity to benzo(a)pyrene. PEF values are presented in Table C-1. The cPAH is calculated as the sum of each individual PAH concentration multiplied by the corresponding PEF value. When the individual PAH component concentration is reported as non-detected, then the PEF is multiplied by half the RL.

**Table C-1. cPAH TEF values**

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

cPAH – carcinogenic polycyclic aromatic hydrocarbon  
PEF – potency equivalency factor

## REFERENCES

- California EPA. 2002. Air Toxics Hot Spots Program Risk Assessment Guidelines, Part II Technical Support Document for Describing Available Cancer Potency Factors. California Environmental Protection Agency, Office of Environmental Health Hazard Assessment.
- Ecology. 2001. Model Toxics Control Act Cleanup Regulation, Chapter 173-340 WAC. Publication No. 94-06. Toxics Cleanup Program, Washington State Department of Ecology, Olympia, WA.