APPENDIX B. DATA MANAGEMENT

Appendix B Data Management

B.1 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 concentrions or reporting limits (RLs) for non-detected 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 concentrationss 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.

B.2 SIGNIFICANT FIGURES AND ROUNDING

The laboratory reports 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.

B.3 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.

B.4 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.

B.5 CALCULATING TOTALS

Total PCB congeners are calculated using only detected values for the 209 PCB congeners. For individual samples in which none of the congeners are detected, the total is given a value equal to the highest RL of the indivual PCB congeners and assigned a U-qualifier indicating the lack of detected concentrations.

B.6 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. 1998; 2006) for mammals as presented in Table B-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 undetected, then the TEF is multiplied by zero, half the RL or the full RL, depending on the calculation method specified.

Table B-1. PCB congener TEF values for mammals

PCB CONGENER NUMBER	WHO 1998 TEF VALUE (UNITLESS)	WHO 2005 TEF VALUE (UNITLESS)
77	0.0001	0.0001
81	0.0001	**0.0003**
105	0.0001	**0.00003**
114	0.0005	**0.00003**
118	0.0001	**0.00003**
123	0.0001	**0.00003**
126	0.1	0.1
156	0.0005	**0.00003**
157	0.0005	**0.00003**
167	0.00001	**0.00003**
169	0.01	**0.03**
189	0.0001	**0.00003**

Bold values indicate a change in TEF value.

B.7 REFERENCES

Van den Berg M, Birnbaum L, Bosveld ATC, Brunström B, Cook P, Feeley M, Giesy JP, Hanberg A, Hasegawa R, Kennedy S, Kubiak T, Larsen JC, van Leeuwen FXR, Djien Liem AK, Nolt C, Peterson RE, Poellinger L, Safe S, Schrenk D, Tillitt D, Tysklind M, Younes M, Waern F, Zacharewski T. 1998. Toxic equivalency factors (TEFs) for PCBs, PCDDs, PCDFs for humans and wildlife. Environ Health Perspec 106(12):775-792.

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.