APPENDIX L – DATA RULES

FIELD AND DATA REPORT

DOWNTOWN PORTLAND
SEDIMENT CHARACTERIZATION

WILLAMETTE RIVER
PORTLAND, OREGON

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PORTLAND HARBOR RI/FS

TECHNICAL MEMORANDUM

GUIDELINES FOR DATA REPORTING, DATA AVERAGING, AND TREATMENT OF NON-DETECTED VALUES FOR THE ROUND 1 DATABASE

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1.0 Introduction

This technical memorandum presents the rules to be followed for development of the Round 1 Site Characterization and Risk Assessment (SCRA) Database from the Round 1 Main Database. The Round 1 Main Database will include all data submitted by the analytical laboratories for analyses conducted on samples collected during the Round 1 field sampling program. The Round 1 Main Database will be maintained so that a data user may examine all the data as reported by the laboratories. Modifications will be made to the Main Database by Integral Consulting, Inc. (Integral) to develop the Round 1 SCRA Database to address the following data issues:

1. Reporting of multiple results for the same constituent in the same sample
2. Reduction of field and laboratory replicates, duplicates, and splits of samples to derive one value for use.

Development of the Round 1 SCRA Database will provide consistency among users of the data for site characterization, ecological risk assessment, and human health risk assessment. Subsequent data reduction conducted by data users (e.g. exposure point concentrations, organic carbon normalized concentrations) will be documented in the associated report or technical memorandum. Rules to be applied in development of the Round 1 SCRA Database are described in the following sections.

2.0 Criteria for Selection of a Value from Multiple Results for the Same Chemical in a Sample

There are several scenarios for sediment and tissue analysis that resulted in the reporting of results for a specific parameter by more than one method:

- A subset of semivolatile organic compound (SVOC) (sediment and tissue) and volatile organic compound (VOC) (sediment) analytes was analyzed by full-scan (EPA Methods 8270 and 8260) and by selected ion monitoring (SIM).
- Selected analytes (hexachlorobutadiene, hexachlorobenzene, hexachloroethane, pentachlorophenol, naphthalene, 1,2,4-trichlorobenzene, 1,2-dichlorobenzene, 1,3-dichlorobenzene, 1,4-dichlorobenzene, aluminum, manganese) were reported by the laboratories by more than one method, as required in the Round 1 quality assurance project plan (QAPP).
- Chlorinated pesticide reanalysis was performed for selected samples.

The following scheme will be used to select the results for parameters being reported by more than one method.

- For VOC and SVOC full-scan and SIM analyses, the highest detected value will be selected for detected results. If results are reported as undetected by both methods, the undetected result with the lowest reporting detection limit (RDL) will be selected for reporting. The SIM analytical technique is more sensitive, and the undetected results were reported at a lower RDL by SIM than by the full-scan method. If one result is detected and one result is undetected, the detected result will be selected for reporting.
- The highest detected naphthalene, 1,2,4-trichlorobenzene, 1,2-dichlorobenzene, 1,3-dichlorobenzene, and 1,4-dichlorobenzene results by EPA Methods 8260B or 8270C will be selected for detected results. If results are reported as undetected by both methods, the 8260B results will be reported because the laboratory RDLs for analysis of these parameters by 8260B are significantly lower than the RDLs for 8270C.
- Hexachlorobutadiene, hexachloroethane, and hexachlorobenzene results were reported by EPA Method 8081A, EPA Method 8270C full-scan, EPA Method 8270C SIM and EPA Method 8270C-ion trap (selected samples). EPA Method 8081A results will be selected for undetected results or results that are not qualified as tentatively identified (NJ qualifier). Method 8081A will be considered the primary analysis because the laboratory RDLs for analysis of these parameters by 8081A are significantly lower than the RDLs for analysis of these parameters by 8270C. However, if the 8081A result for these parameters was qualified as tentatively identified (N or NJ qualifier), the undetected result with the lowest RDL (GC/MS SIM or GC/MS ion trap) will be selected for reporting.
- Pentachlorophenol was analyzed by three methods for sediment: 8151, 8270C full-scan, and 8270C SIM. However, the laboratory encountered problems with low matrix spike recoveries for pentachlorophenol by EPA Method 8151. Therefore, results by EPA Method 8151 were not included in the evaluation of results selected for reporting for pentachlorophenol. The highest detected result from the 8270C full-scan and 8270C SIM analyses will be reported for detected results. If results are reported as undetected by both methods, the undetected result with the lowest RDL will be selected for reporting. If one result is detected and one result undetected, the detected result will be selected for reporting. For tissue samples, pentachlorophenol was reported by two methods: 8270C and 8270C SIM. The SIM result is preferred because the reporting limit for the SIM analysis is typically an order of magnitude lower than the reporting limit for the analysis by 8270C full-scan.
- Aluminum and manganese in selected sediment samples were analyzed by EPA methods 6010B and 6020. The highest detected value will be selected for detected results. If results are reported as undetected by both methods, the undetected result with the lowest RDL will be selected for

reporting. If one result is detected and one result is undetected, the detected result will be selected for reporting. The remaining sediment samples were analyzed for aluminum and manganese by EPA Method 6010B.

2.1 SELECTION OF CHLORINATED PESTICIDE RESULTS

The LWG's recommendations for selection of chlorinated pesticide results were included in a May 7, 2004 Technical Memorandum (Finalization of Round 1 Chlorinated Pesticide Data). The selection of chlorinated pesticide results was resolved cooperatively with EPA and its partners. The selection criteria for reporting of chlorinated pesticide results are presented below.

Of the two methods used to analyze for pesticides, GC/ECD provides greater sensitivity and GC/MS provides greater selectivity. In order to obtain the greatest benefit from each method, data were selected for reporting based on their detection status and qualification status. A set of rules was developed to select which result to report for each sample, as described below:

1. The analyte is not detected by either method: Report the lowest reporting limit.
2. The analyte is detected by GC/ECD but undetected by GC/MS-ion trap: Evaluate the qualifiers and the magnitude of the analyte concentration (GC/ECD) with respect to the reporting limit (GC/MS-ion trap).
    a. The GC/ECD result is qualified N or NJ: Report the GC/MS-ion trap reporting limit.
    b. The GC/ECD result is higher than the GC/MS-ion trap reporting limit and is not qualified N or NJ: Report the average of the GC/ECD result and the GC/MS-ion trap reporting limit without a U (i.e., the analyte is reported as detected).
    c. The GC/ECD result is lower than the GC/MS-ion trap reporting limit and is not qualified N or NJ: Report the GC/ECD result.
3. The analyte is undetected by GC/ECD but detected by GC/MS-ion trap: Report the GC/MS-ion trap result.
4. The analyte is detected by both methods: Evaluate the qualifiers.
    a. The GC/ECD result is qualified N or NJ: Report the GC/MS-ion trap result.
    b. Either or both results are qualified J or unqualified: Report the average of the results for GC/ECD and GC/MS-ion trap; apply a J qualifier if one or both results are J-qualified.

Matrix interference that resulted in elevated reporting limits for many of the target chlorinated pesticide compounds was encountered for five of the smallmouth bass samples in the Method 8270C analysis. To resolve this interference, these five

sample extracts were subjected to acid cleanup. Selected target compounds (i.e., beta-endosulfan, dieldrin, endosulfan sulfate, endrin, endrin aldehyde, endrin ketone, and methoxychlor), were not recovered after acid cleanup, as indicated by the recoveries of these compounds in the laboratory quality control samples. Results for these compounds from the extract prior to acid cleanup, with an elevated reporting limit, were evaluated against the selection criteria. The remaining target compounds were successfully recovered from the acid extract, and the results from the acid cleanup extract were evaluated against the selection criteria.

2.2 REPORTING OF PCB CONGENER COELUTIONS

Coeluting PCB congeners were reported by the analytical laboratory as individual results, where the first congener of a coelution was reported with the quantitative value and a C qualifier. The other congeners in a coelution were reported with only a C qualifier and the PCB number of the first congener to refer the data user back to that congener for the quantitative value of the coelution. For example, PCB 90, PCB 101, and PCB 113 coeluted, so if the value of that coelution was 37, then PCB 90 was reported by the laboratory as "37 C," PCB 101 was reported as "C90," and PCB 113 was reported as "C90."

In the database, the records of individual congeners in coelutions will be replaced with a single record that has a parameter name that includes the PCB numbers of each of the coeluting congeners. In the above example, the records for PCB 90, PCB 101, and PCB 113 will be replaced with a single record containing the parameter name "PCB 90,101,113" and the quantitative value "37."

3.0 DATA REDUCTION FOR DEVELOPMENT OF SCRA DATABASE

Field duplicate, triplicate, and split samples were collected for selected tissue and sediment samples during the Round 1 field investigation, as required by the QAPP. In addition, duplicates were generated by the laboratory for metals analyses and some conventional parameters, as required by the associated analytical method. Therefore, there are multiple results for selected field samples due to the collection and analysis of field and laboratory duplicates and replicates. Duplicate, triplicate, and split samples (field and laboratory) will be reported as individual results in the Round 1 Main Database. The sample type field will indicate that the result is a duplicate, triplicate, or split, and the parent sample will be identified in another field.

For data interpretation purposes, the process described in the following sections will be used to calculate a single concentration for a parameter for which field or laboratory duplicates, replicates, or splits resulted in multiple results for a specific parameter at a field location. The data reduction activities described below will occur after data validation is complete in order to incorporate data qualifiers applied during

validation. The single concentration resulting from the data reduction activities will be included in the Round 1 SCRA Database.

3.1 TREATMENT OF NON-DETECTED VALUES IN AVERAGES

If a chemical is not detected in a sample, the result will be represented in the database as the RDL and a laboratory qualifier such as U, UJ, etc. in the laboratory qualifier field. A "detect flag" field will be populated with a Y for detected values and an N for non-detects. Non-detected values will be incorporated into duplicates and sums according to the rules in the following sections.

3.2 LABORATORY DUPLICATES

Laboratory duplicates for sediment and tissue samples will be averaged as described below:

- When averaging laboratory duplicates, assume that the data validation qualifiers assigned to the field sample are also assigned to the associated laboratory duplicate results and then implement the steps identified in the following bullets.
- If the sample and laboratory duplicate results are both reported as detected concentrations, the average concentration will be calculated and used in all further data reduction activities.
- If the sample and laboratory duplicate results are both reported as undetected, the lower RDL for the two undetected results will be selected and designated a non-detect for use in all further data reduction activities.
- If either the sample or laboratory duplicate result is reported as detected and the associated sample or laboratory duplicate result is reported as undetected, the detected result will be selected for reporting and will be used in all further data reduction activities.

3.3 FIELD SPLIT AND REPLICATE RESULTS FOR SEDIMENT SAMPLES

Field split samples were collected for sediment samples by collecting two aliquots of the sediment composite sample and submitting both aliquots for laboratory analysis. Field replicate samples were also collected for sediment samples by collecting three samples from the same station and submitting the three samples from the station for laboratory analysis. Field replicate results will be retained in the SCRA database as individual sample results. Field split samples will be averaged as described below:

- If the sample and field split results are all reported as detected concentrations, the average concentration will be calculated and used in all further data reduction activities.

- If the sample and field split results are all reported as undetected, the lowest RDL for the undetected results will be selected and designated a non-detect for use in all further data reduction activities.
- If the sample and field split results are mixed (i.e., one is reported as detected and one is reported as undetected), the detected result will be selected for reporting and used in all further data reduction activities.

3.4 FIELD REPLICATE RESULTS FOR TISSUE SAMPLES

Field replicate samples were generated for tissue samples by collecting additional fish in the field and generating two or three composite samples for each replicate station. The composite samples were generated by homogenizing up to five individual fish (or about 350 grams for crayfish and sculpin samples) for each composite sample. Because the field replicate samples for tissue were generated by compositing separate individual fish, the fish field replicate samples will be treated as separate samples.

3.5 HIERARCHY FOR CALCULATION OF AVERAGE CONCENTRATIONS

Selected sediment samples have associated laboratory duplicate, field split, and field replicate results. In these cases, the average concentrations will be calculated in the following order:

- Laboratory duplicates will be evaluated first, and the resulting average or selected value will be used in the following step.
- Field splits will be evaluated next and the resulting average or selected value will be used in the following step.
- Field replicates will be retained in the SCRA database as individual sample results. However, subsequent data evaluation may result in averaging of the field replicate results.

3.6 PROPAGATION OF QUALIFIERS IN CALCULATED AVERAGES

In cases where multiple results are generated due to analysis of duplicates, and splits, and average concentrations are derived as described above, it is necessary to define how the data validation qualifiers will be assigned to the calculated average concentrations. Data validation qualifiers will be propagated as follows:

- If all results included in the calculated average are qualified with the same qualifier (e.g., U or J), then this qualifier will be applied to the calculated average.
- If one or more of the results are qualified as undetected and one or more of the other results included in the average are detected and qualified as estimated, the calculated average will be qualified as estimated.

- If all of the included results are detected and one or more of the results is qualified as estimated, the calculated average will be qualified as estimated.
- As noted above, a "detect flag" field will be populated with a Y for detected values and an N for non-detects for all samples and calculated averages in both the Round 1 Main Database and the Round 1 SCRA Database.
- A T qualifier will be added to all results in the SCRA database that are mathematically derived (e.g., from calculating the average of multiple results) and all results that are selected for reporting in preference to other available results (e.g., for parameters reported by multiple methods) for the Round 1 data.

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ROUND 3B SEDIMENT DATA REPORT

APPENDIX F

SUMMATION RULES AND SCRA DATABASE, EXCEL FLAT FILE FORMAT

(FOUND ON ACCOMPANYING CD)

DRAFT

DO NOT QUOTE OR CITE
This document is currently under review by US EPA and its federal, state, and tribal partners, and is subject to change in whole or in part.

August 1, 2008

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1.0 CALCULATED TOTALS

Calculated totals were created for analytes evaluated on the basis of summed concentrations. The calculated totals include: total PCB Aroclors, total PCB congeners, total PAH, total low-molecular-weight PAH (LPAH), total high-molecular-weight PAH (HPAH), total DDD, total DDE, total DDT, total DDx, total chlordanes, total endosulfans, total xylenes, total benzene + toluene + ethylbenzene + xylene (BTEX), total fines, TPH, and total PCDD/Fs. All totals were either T or A qualified to indicate that the values were manipulated values (i.e., summed or selected). The A qualifier was used when all of the individual analytes necessary for the total were not available (i.e., a partial sum).

1.1 GENERAL SUMMATION RULES

Calculated totals are the sum of all detected concentrations. If all of the analytes were not detected, then the highest reporting detection limit was the selected value for the calculated total, and a U qualifier was added to indicate the lack of detected values.

1.2 CALCULATED TOTALS

Total PCBs were calculated two ways: as total PCB Aroclors and as total PCB congeners. Total PCB Aroclors represented the sum of Aroclors. Total PCB congeners represented the sum of the individual congeners.

Total LPAHs were calculated with the concentrations for 2-methylnaphthalene, acenaphthene, acenaphthylene, anthracene, fluorene, naphthalene, and phenanthrene. Total HPAHs were calculated with the concentrations for fluoranthene, pyrene, benzo(a)anthracene, chrysene, benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3,-c,d)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene. Total PAHs were calculated with the concentrations of the individual LPAHs and HPAHs.

Total DDx were calculated with the concentrations of the six DDx compounds: 2,4′-DDD; 4,4′-DDD; 2,4′-DDE; 4,4′ DDE; 2,4′-DDT; and 4,4′-DDT. Total DDD were calculated with 2,4′-DDD and 4,4′-DDD; total DDE were calculated with 2,4′-DDE and 4,4′-DDE; and total DDT were calculated with 2,4′-DDT and 4,4′-DDT.

Total chlordanes were calculated as the sum of the following compounds: cis-chlordane, trans-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor.

Total endosulfans were calculated as the sum of alpha-endosulfan, beta-endosulfan, and endosulfan sulfate.

Total xylenes were calculated as the sum of m,p-xylene and o-xylene.

BTEX were calculated as the sum of benzene, toluene, ethylbenzene, and xylenes.

Total fines were calculated as the sum of all silt and clay grain-size fractions passing U.S. standard sieve #230 (0.0625-mm openings).

Total petroleum hydrocarbons were calculated as the sum of diesel-range hydrocarbons, residual-range hydrocarbons, and gasoline-range hydrocarbons.

Total PCDD/Fs were calculated as the sum of dioxin and furan homologs: tetrachlorodibenzo-p-dioxins, pentachlorodibenzo-p-dioxins, hexachlorodibenzo-p-dioxins, heptachlorodibenzo-p-dioxins, octachlorodibenzo-p-dioxin, tetrachlorodibenzofurans, pentachlorodibenzofurans, hexachlorodibenzofurans, heptachlorodibenzofurans, and octachlorodibenzofuran.

1.3 CALCULATION OF TOXICITY EQUIVALENTS

1.3.1 Calculation of PCB Congener TEQs

PCB congener toxic equivalents (TEQs) were calculated using the 2005 World Health Organization (WHO) consensus toxic equivalency factor (TEF) values for mammals (Van den Berg et al. 2006). TEQs were calculated as the sum of each congener concentration (or detection limit for non-detects) multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied times the TEF value.

1.3.2 Calculation of Dioxin and Furan TEQs

Dioxin and furan TEQs were calculated using the 2005 WHO consensus TEF values for mammals (Van den Berg et al. 2006). TEQs were calculated as the sum of each congener concentration (or detection limit for non-detects) multiplied by the corresponding TEF value. When all of the congeners were not detected in a given sample, then the reported TEQ value was the highest congener detection limit multiplied time the TEF value.

1.4 SIGNIFICANT FIGURES

The laboratories provided results in electronic text files. The text values were maintained in the database so that the number of significant figures provided by the

labs would not be lost by either the addition or removal of trailing zeros. For example, if the lab file contained 1.0, then that text string would be maintained to avoid conversion to either 1.00 or 1. In some cases, the lab reported value appeared to have only one significant figure (1, for example). But a minimum of two significant figures was assumed for all results, which was consistent with the standard reporting requirements of analytical laboratories.

During calculations, such as averaging replicates or summing for totals, all significant figures were carried through the calculation. The final result was then rounded to the smallest number of significant figures found in the values used in the calculation. For example: 7010 + 105 + 20.8 = 7135.8, and with three significant figures equals 7140.

2.0 REFERENCES

Van den Berg, M. L.S. Birnbaum, M. Denison, M. De Vito, W. Farland, M. Freeley, H. Fiedler, H. Hakansson, A. Hanberg, L. Haws, M. Rose, S. Safe, D. Schrenk, C. Tohyama, A. Tritscher, J. Tuomisto, M. Tysklind, N. Walker, and R.E. Peterson. 2006. The 2005 World Health Organization Reevaluation of Human and Mammalian Toxic Equivalency Factors for Dioxins and Dioxin-Like Compounds. Toxicological Sciences 93(2), 223-241.