PORTLAND HARBOR RI

# APPENDIX G
# BASELINE ECOLOGICAL RISK ASSESSMENT

## ATTACHMENT 3
## DATA MANAGEMENT

**DRAFT**

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August 19, 2009

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# 1.0 BERA DATASET

The LWG sampling events and non-LWG sampling events included in the site characterization and risk assessment (SCRA) dataset are described in detail in Section 2.0 of the draft remedial investigation (RI). This attachment presents the data management rules used to reduce and refine the SCRA dataset into the baseline ecological risk assessment (BERA) dataset used in this risk analysis. The data management rules (including data reduction, data usability, and data quality) used to develop the SCRA dataset are described in detail in Section 2.0 of the draft RI.

The BERA dataset includes only those matrices relevant for ecological exposure pathways: surface (0 to 30 cm) sediment, benthic invertebrate and fish tissue of multiple aquatic species, surface water, and shallow (0 to 38 cm) transition zone water (TZW). These data were collected over multiple rounds of sampling from throughout the Study Area and include both LWG- and non-LWG-collected data from the sampling period of 1997 to 2007. A summary of the data used in the BERA dataset is presented in Section 4.0 of the BERA.

The following data reduction tasks were conducted on the BERA data and are described in this attachment:

- Derivation of chemical group totals
- Organic carbon (OC)-normalization
- Derivation of toxicity equivalency (TEQ) concentrations
- Calculation of steady-state concentrations extrapolated from laboratory-exposed tissue concentrations
- Treatment of significant figures
- Treatment of field replicates
- Reconciliation of different water sampling methods

# 2.0 CALCULATED TOTALS

This section presents the summation rules and the calculation of totals for selected chemical groups. Calculated totals were created for analytes evaluated on the basis of summed concentrations. The calculated total concentrations include: total polychlorinated biphenyls (PCBs) (as Aroclors or congeners[1]), polycyclic aromatic hydrocarbon (PAHs), low-molecular-weight PAHs (LPAHs), high-molecular-weight PAHs (HPAHs), sum DDD, sum DDE, sum DDT, total DDx (sum of all six DDT isomers [2,4′-DDD, 4,4-DDD, 2,4′-DDE, 4,4-DDE, 2,4′-DDT and 4,4′-DDT]), total chlordane, total endosulfan, and total xylene. The following subsections present the data rules used to calculate totals in the BERA dataset.

## 2.1 DETERMINING THE PRESENCE OF AN INDIVIDUAL ANALYTE

The determination of whether to include an individual analyte (e.g., a PCB congener) in a calculated chemical group sum (e.g., total PCBs) was based on whether it was detected within the Study Area dataset for each media. For each of the following media, an analyte was considered to be present if it was detected at least once within the Study Area:

- Surface water
- TZW
- Surface sediment
- Fish tissue
- Invertebrate tissue

If an analyte was not detected in any sample of a given medium, then the analyte was considered not present, and the non-detected values were excluded from the calculated sum.

## 2.2 GENERAL SUMMATION RULES

Calculated totals are the sum of all detected concentrations; non-detected results are included based on the following rules for each medium (i.e., surface water, TZW, sediment, fish tissue, or benthic invertebrate tissue):

- Non-detects for individual analytes detected at least once within a given medium were included in the summation for that media using one-half the detection limit (DL).
- Non-detects for individual analytes that were never detected within a given medium were not included in the summation (Table 2-1).

[1] Total PCBs were calculated based on the sum of Aroclors or the sum of 209 congeners. Section 2.3 presents how the total PCB concentration was represented in a given sample in which both PCB Aroclors and PCB congeners were analyzed.

- If all of the analytes were not detected within a given sample, then the highest DL for any of the group constituents was the selected value for the calculated total. The total was qualified with a "U" to indicate the lack of detected values.

Table 2-1. Analytes Excluded from Total Calculation Because They Were Not Detected in the BERA Dataset

| Calculated Total | Excluded Analytes |
|---|---|
| **Sediment** | |
| Total PCBs (Aroclors) | Aroclor 1232, Aroclor 1262 |
| **Benthic Tissue** | |
| Total PCBs (Aroclors) | Aroclor 1016, Aroclor 1221, Aroclor 1232, Aroclor 1242, Aroclor 1254, Aroclor 1262, Aroclor 1268 |
| Total PCBs (congeners) | PCB 078, PCB 161, PCB 192 |
| **Fish Tissue** | |
| Total PCBs (Aroclors) | Aroclor 1016, Aroclor 1221, Aroclor 1242, Aroclor 1254, Aroclor 1262, Aroclor 1268 |
| Total PCBs (congeners) | PCB 192 |
| **Surface Water** | |
| Total PCBs (Aroclors) | Aroclor 1016, Aroclor 1221, Aroclor 1232, Aroclor 1242, Aroclor 1262, Aroclor 1268 |
| Total PCBs (congeners) | PCB 161 |
| **Transition Zone Water – Shallow** | |
| Total DDx | 2,4′-DDE |

BERA – baseline ecological risk assessment
DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
PCB – polychlorinated biphenyl
Total DDx – sum of all six DDT isomers (2,4′-DDD; 4,4′-DDD; 2,4′-DDE; 4,4′-DDE; 2,4′-DDT; and 4,4′-DDT)

In order to ensure that the sums were always calculated based on comparable datasets, the number of group components available (i.e., analyzed for) was evaluated prior to summing. The number of analytes varied because the sample was analyzed for a subset of a chemical group (i.e., analysis of a subset of congeners rather than the complete list) or because individual analytical results were removed due to quality assurance concerns.

The minimum number of analytes required for the calculation of each total is summarized in Table 2-2. If the number of analytes was limited, then the total was calculated but qualified with an "A" to indicate that there were analytes unavailable for summation. If too few analytes were available, then the total was not calculated. Only one sediment sample was found to have an insufficient number of analytes for the calculation of total PCBs (based on Aroclors). This sample was analyzed for only one Aroclor. Ninety-eight sediment samples were determined to have insufficient congener data for the calculation of total PCBs (based

on congeners). These samples were analyzed for a limited group of congeners, which represented a small subset of the total PCB concentrations for these samples. Sixty-seven TZW samples, twenty-three surface water samples, and one sediment sample were analyzed only for one PAH compound, naphthalene; therefore, total LPAH and total PAH values were not calculated for these samples.

Table 2-2. Number of Analytes Required for Each Calculated Total

| Calculated Total | Maximum Number of Analytes | Limited Number of Analytes (A-qualified) | Insufficient Number of Analytes (no sum calculated) | Number of Samples with No Sum |
|---|---|---|---|---|
| Total PCBs (Aroclors) | 7 or 9 | < 7 | < 2 | 1 sediment |
| Total PCBs (congeners) | 209 | < 150 | < 100 | 98 sediment |
| Total HPAHs | 10 | < 10 | < 5 | none |
| Total LPAHs | 7 | < 7 | < 3 | 67 TZW, 23 SW, 1 sediment |
| Total PAHs | 17 | < 17 | < 10 | 67 TZW, 23 SW, 1 sediment |
| Sum DDD | 2 | < 2 | NA | none |
| Sum DDE | 2 | < 2 | NA | none |
| Sum DDT | 2 | < 2 | NA | none |
| Total DDx | 6 | < 6 | NA | none |
| Total chlordane | 5 | < 5 | NA | none |
| Total endosulfan | 3 | < 3 | NA | none |
| Total xylene | 3 | < 2 | NA | none |

DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
HPAH – low-molecular-weight polycyclic aromatic hydrocarbon
LPAH – high-molecular-weight polycyclic aromatic hydrocarbon
NA – not applicable
PAH – polycyclic aromatic hydrocarbon
PCB – polychlorinated biphenyl
Total DDx – sum of all six DDT isomers (2,4′-DDD; 4,4′-DDD; 2,4′-DDE; 4,4′-DDE; 2,4′-DDT; and 4,4′-DDT )
TZW – transition zone water
SW – surface water

## 2.3 INDIVIDUAL ANALYTES IN CALCULATED TOTALS

Total PCBs were calculated based on the sum of Aroclors or the sum of 209 congeners. The total PCB concentration is represented as follows for each of the BERA datasets.[2]

[2] PCBs were not analyzed in TZW.

- For all BERA surface sediment samples, the total PCB concentration is represented by total PCB Aroclors.
- For the BERA tissue dataset, the total PCB concentration is represented by total PCB Aroclors for Round 1 samples and total PCB congeners for Round 2 and Round 3 samples. Aroclors were selected over congeners for Round 1 because PCB congener analysis was performed on only a limited number of samples.
- For the BERA surface water dataset, the total PCB concentration is represented by total PCB congeners for all XAD samples and by total PCB Aroclors for locations where only peristaltic samples were collected.

Total LPAHs are the sum of concentrations of naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, and 2-methylnaphthalene. Total HPAHs are the sum of concentrations for fluoranthene, pyrene, benzo(a)anthracene, chrysene, total benzofluoranthenes, benzo(a)pyrene, indeno(1,2,3-cd)pyrene, dibenzo(a,h)anthracene, and benzo(g,h,i)perylene. Total PAHs are the sum of LPAHs and HPAHs.

Total DDx are the sum the six DDT isomers: 2,4′-DDD; 4,4′-DDD; 2,4′-DDE; 4,4′-DDE; 2,4′-DDT; and 4,4′-DDT. The sum DDD was the sum of 2,4′-DDD and 4,4′-DDD, the sum DDE was the sum of 2,4′-DDE and 4,4′-DDE, and the sum DDT was the sum of 2,4′-DDT and 4,4′-DDT.

Total chlordane was calculated as the sum of the following compounds: cis-chlordane, trans-chlordane, oxychlordane, cis-nonachlor, and trans-nonachlor. Total endosulfan was calculated as the sum of alpha-endosulfan, beta-endosulfan, and endosulfan sulfate. Total xylene was calculated as the sum of m,p-xylene, o-xylene, and xylene.

# 3.0 ORGANIC CARBON NORMALIZATION

This section presents the organic carbon normalization process used in the SLERA (Section 3.1) and in the BERA (Section 3.2).

## 3.1 ORGANIC CARBON NORMALIZATION IN THE SLERA

In the SLERA, the organic carbon-normalized concentration for each non-polar organic analyte in the sediment dataset was calculated as follows:

- The fractional organic carbon content, $f_{oc}$ (TOC%/100), was used for all calculations
- Organic carbon-normalized values were calculated as $C_{dw}/f_{oc}$ , where $C_{dw}$ is the dry-weight concentration in mg/kg
- For total organic carbon (TOC) below 0.2%, the TOC value was substituted with 0.2%; for missing values, the TOC value was substituted with 1.0%.
- No upper TOC limit that would exclude normalization was set.

## 3.2 ORGANIC CARBON NORMALIZATION IN THE BERA

In the BERA the organic carbon-normalized concentration for each organic analyte in the sediment dataset was calculated as follows:

- The fractional organic carbon content, $f_{oc}$ (TOC%/100) was used for all calculations
- Organic carbon-normalized values were calculated as $C_{dw}/f_{oc}$, where $C_{dw}$ is the dry-weight concentration in mg/kg
- No upper TOC limit that would exclude normalization was set; however, for higher TOC values (> 4.0%), each individual sample was evaluated for possible anthropogenic contributions to organic carbon (e.g., wood waste, petroleum, non-aqueous-phase liquids [NAPLs], or sewage) that may have confounded partitioning assumptions.
- For TOC < 0.2% or high values with contribution from anthropogenic wastes (see previous bullet), no OC-normalized value was calculated. In these few cases, sample data were evaluated on a dry weight basis only
- For samples without TOC data, the value was estimated using a regression equation based on site-specific TOC and grain size (as percent fines) from the Upriver Reach (above River Mile [RM] 15.3).

# 4.0 CALCULATION OF TOXICITY EQUIVALENTS

TEQs were calculated for dioxin-like PCB congeners and dioxin and furans A TEQ is the sum of the constituents (i.e., toxicity equivalence concentrations [TECs]), representing a total dioxin concentration, modified by factors reflecting the toxicity of each constituent relative to the most toxicity constituent (2,3,7,8-tetrachlorodibenzo-*p*-dioxin). TECs were calculated consistent with EPA guidance (EPA 2008). Toxicity equivalency factors (TEFs) are based on the World Health Organization (WHO) values for fish and birds (Van den Berg et al. 1998) and mammals (Van den Berg et al. 2006), as presented in Tables 4-1 and 4-2. TEQs were calculated if at least one TEQ constituent for a given sample was detected using the following method:

- If an analyte was detected (D), the concentration was multiplied by the TEF in the sum.
- If an analyte was not detected (ND) but determined to be present in the BERA dataset, one-half the DL was multiplied by the TEF in the sum.
- If an analyte was ND and determined not to be present in the BERA dataset, the value of zero was used in sum.
- If all analytes used to create a TEQ were ND, the maximum toxicity-weighted DL was reported as the TEQ, and the result was flagged with a "U."

**Table 4-1. Dioxin-like PCB Congener TEFs**

| Congener Number | TEF Values (unitless) | | |
|---|---|---|---|
| | Fish[a] | Birds[a] | Mammals[b] |
| PCB 77 | 0.0001 | 0.05 | 0.0001 |
| PCB 81 | 0.0005 | 0.1 | 0.0003 |
| PCB 105 | < 0.000005 | 0.0001 | 0.0003 |
| PCB 114 | < 0.000005 | 0.0001 | 0.0003 |
| PCB 118 | < 0.000005 | 0.00001 | 0.0003 |
| PCB 123 | < 0.000005 | 0.00001 | 0.0003 |
| PCB 126 | 0.005 | 0.1 | 0.1 |
| PCB 156 | < 0.000005 | 0.0001 | 0.0003 |
| PCB 157 | < 0.000005 | 0.0001 | 0.0003 |
| PCB 167 | < 0.000005 | 0.00001 | 0.0003 |
| PCB 169 | 0.00005 | 0.001 | 0.03 |
| PCB 189 | < 0.000005 | 0.00001 | 0.0003 |

[a] Fish and bird TEFs based on Van den Berg et al. (1998).
[b] Mammal TEFs based on Van den Berg et al. (2006).
PCB – polychlorinated biphenyl
TEF – toxic equivalency factor

**Table 4-2. Dioxin and Furan TEFs**

| Dioxin and Furan Congeners | TEF Values (unitless) | | |
|---|---|---|---|
| | Fish[a] | Birds[a] | Mammals[b] |
| 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin | 1 | 1 | 1 |
| 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin | 1 | 1 | 1 |
| 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin | 0.5 | 0.05 | 0.1 |
| 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin | 0.01 | 0.01 | 0.1 |
| 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin | 0.01 | 0.1 | 0.1 |
| 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin | 0.001 | < 0.001 | 0.01 |
| Octachlorodibenzodioxin | < 0.0001 | 0.0001 | 0.0003 |
| 2,3,7,8-Tetrachlorodibenzofuran | 0.05 | 1 | 0.1 |
| 1,2,3,7,8-Pentachlorodibenzofuran | 0.05 | 0.1 | 0.03 |
| 2,3,4,7,8-Pentachlorodibenzofuran | 0.5 | 1 | 0.3 |
| 1,2,3,4,7,8-Hexachlorodibenzofuran | 0.1 | 0.1 | 0.1 |
| 1,2,3,6,7,8-Hexachlorodibenzofuran | 0.1 | 0.1 | 0.1 |
| 1,2,3,7,8,9-Hexachlorodibenzofuran | 0.1 | 0.1 | 0.1 |
| 2,3,4,6,7,8-Hexachlorodibenzofuran | 0.1 | 0.1 | 0.1 |
| 1,2,3,4,6,7,8-Heptachlorodibenzofuran | 0.01 | 0.01 | 0.01 |
| 1,2,3,4,7,8,9-Heptachlorodibenzofuran | 0.01 | 0.01 | 0.01 |
| Octachlorodibenzofuran | < 0.0001 | 0.0001 | 0.0003 |

[a] Fish and bird TEFs based on Van den Berg et al. (1998).
[b] Mammal TEFs based on Van den Berg et al. (2006).
NA – not available
TEF – toxic equivalency factor

The TEFs used to calculate TEQs for dioxin-like PCB congeners were WHO consensus values for fish and birds from Van den Berg et al. (1998) and the updated WHO mammal TEFs from Van den Berg et al. (2006). The rationale for the use of TEFs is based on evidence that there is a common mechanism of toxicity for certain dioxins, furans, and PCB congeners, which involves binding to the aryl hydrocarbon (Ah) receptor as an initial step. Data on the relative binding affinity of particular PCB congeners compared to 2,3,7,8-TCDD are available from *in vivo* and *in vitro* studies. These data have been used to derive TEFs for PCB congeners that show structural similarity to dioxins, bind to the Ah receptor, and elicit dioxin-specific biochemical and toxic responses.

A key uncertainty in the TEQ approach is related to the derivation of consensus TEF values. Limitations in the underlying data used to derive TEFs, such as the relevance of the endpoints in the studies and the lack of information on interspecies variability, contribute to the uncertainty.

# 5.0 STEADY-STATE ADJUSTMENT OF BENTHIC TISSUE

Field and steady-state conditions may not be represented in tissue concentrations measured in laboratory-exposed *Lumbriculus* and *Corbicula* within the 28-day exposure period. Therefore, detected concentrations of neutral organic chemicals of interest [COIs][3] in lab-exposed worm (*Lumbriculus*) and lab-exposed clam (*Corbicula)* tissue were adjusted to estimate steady-state concentrations using the process based on McFarland (1995) and described in the US Army Corps of Engineers (USACE) inland testing manual (EPA and USACE 1998).

The adjustments for steady state were developed in a series of equations from McFarland (1995), the first of which estimates the time to steady state for a given chemical, based on its partitioning coefficient:

$$\text{Log } t_{ss} = 6.9 \times 10^{-3} (\log K_{ow})^4 - 1.85 \times 10^{-1} (\log K_{ow})^3 - 1.65 (\log K_{ow})^2 - 5.34 (\log K_{ow}) + 5.93$$

**Equation 1**

Where:

$t_{ss}$ = time to reach steady state (days)
$K_{ow}$ = octanol-water partitioning coefficient

The fraction of steady state that a chemical has reached after a defined exposure period is dependent, in part, on the elimination rate ($k_2$), which is calculated as:

$$k_2 = \frac{-\ln(1 - f_{ss})}{t_{ss}}$$

**Equation 2**

Where:

k2 = elimination rate
$f_{ss}$ = assumed fraction of steady state (0.99 from McFarland (1995))
$t_{ss}$ = time to reach steady state (from Equation 1)

For this equation, the value of $f_{ss}$ is near 1.0 (i.e., 0.99) because the approach to steady-state is asymptotic.

The fraction of steady state is then derived from the following equation, using 28 days as the value of *t*:

[3] COIs were determined by evaluating the detection status of each neutral organic chemical in all the benthic tissue data. If a chemical was never detected it was not a COI. The COI determination also affected how the values were handled in the sums; non-detects were included in the sum at one-half DL if they were COIs, otherwise they were treated as 0.

$$f_{ss} = 1 - e^{k_2 t}$$ **Equation 3**

Where:

$f_{ss}$ = fraction of steady state that 28 days represents
e = base e (base of natural log)
$k_2$ = elimination rate (from Equation 2)
t = time (i.e., 28 days)

Finally, the steady-state concentrations was calculated as:

$$C_{ss} = \frac{c_t}{f_{ss}}$$ **Equation 4**

Where:

$C_{ss}$ = estimated concentration in tissue, at steady state
$C_t$ = concentration in tissue after 28 days of exposure
$f_{ss}$ = fraction of steady state that 28 days represents

Adjusted steady-state concentrations were derived for neutral organic COIs, including the following chemical groups: butyltins, PAHs, PCBs, dioxins and furans, phenols, phthalates, SVOCs, and pesticides.

The log $K_{ow}$ of each of the neutral organic COIs were compiled from multiple data sources In addition, it was desirable to use the same partitioning assumptions used in the food web modeling for the BERA. Table 5-1 presents the $K_{OW}$ values and sources used to calculate steady-state adjusted concentrations. For PCB congener coelutions, the average of the log $K_{OW}$ of the coeluting chemicals was used for the coelution. The proportion of the steady-state concentration was calculated for each chemical using the equations and methods presented in McFarland (1995). Each concentration was then adjusted with a factor that was the reciprocal of the decimal fraction indicating the proportion of the steady-state concentration.

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| **Butyltins** | | |
| Butyltin ion | 3.3 | EPI Suite Database (EPA 2007) |
| Dibutyltin ion | 3.3 | EPI Suite Database (EPA 2007) |
| Tetrabutyltin | 3.3 | EPI Suite Database (EPA 2007) |
| Tributyltin ion | 3.3 | EPI Suite Database (EPA 2007) |
| **PAHs** | | |
| 1-Methylnaphthalene | 3.7 | EPI Suite Database (EPA 2007) |
| 2-Methylnaphthalene | 3.7 | EPI Suite Database (EPA 2007) |
| Acenaphthene | 3.9 | McFarland (1995) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| Acenaphthylene | 4.1 | McFarland (1995) |
| Anthracene | 4.3 | McFarland (1995) |
| Benzo(a)anthracene | 5.6 | McFarland (1995) |
| Benzo(a)pyrene | 6.0 | McFarland (1995) |
| Benzo(b)fluoranthene | 6.1 | EPI Suite Database (EPA 2007) |
| Benzo(e)pyrene | 6.1 | EPI Suite Database (EPA 2007) |
| Benzo(g,h,i)perylene | 7.0 | McFarland (1995) |
| Benzo(k)fluoranthene | 6.1 | EPI Suite Database (EPA 2007) |
| C1-Chrysene | 5.5 | EPI Suite Database (EPA 2007) |
| C1-Dibenzothiophene | 4.2 | EPI Suite Database(EPA 2007) |
| C1-Fluoranthene/pyrene | 5.2 | average[a] |
| C1-Fluorene | 4.0 | EPI Suite Database (EPA 2007) |
| C1-Phenanthrene/anthracene | 4.4 | average[a] |
| C2-Fluoranthene/pyrene | 5.2 | average[a] |
| C2-Fluorene | 4.0 | EPI Suite Database (EPA 2007) |
| C2-Naphthalene | 3.2 | EPI Suite Database (EPA 2007) |
| C2-Phenanthrene/anthracene | 4.4 | average[a] |
| C3-Dibenzothiophene | 4.2 | EPI Suite Database (EPA 2007) |
| C3-Fluorene | 4.0 | EPI Suite Database (EPA 2007) |
| C3-Naphthalene | 3.2 | EPI Suite Database (EPA 2007) |
| C3-Phenanthrene/anthracene | 4.4 | average[a] |
| C4-Naphthalene | 3.2 | EPI Suite Database (EPA 2007) |
| C4-Phenanthrene/anthracene | 4.4 | average[a] |
| Chrysene | 5.6 | McFarland (1995) |
| Dibenzo(a,h)anthracene | 6.0 | McFarland (1995) |
| Dibenzothiophene | 4.2 | EPI Suite Database (EPA 2007) |
| Fluoranthene | 4.9 | EPI Suite Database (EPA 2007) |
| Fluorene | 4.2 | EPA (1994) |
| Indeno(1,2,3-cd)pyrene | 6.7 | EPI Suite Database (EPA 2007) |
| Naphthalene | 3.4 | EPA (1994) |
| Perylene | 6.1 | EPI Suite Database (EPA 2007) |
| Phenanthrene | 4.5 | McFarland (1995) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| Pyrene | 4.9 | McFarland (1995) |
| **SVOCs** | | |
| 4-Chloroaniline | 1.7 | EPI Suite Database(EPA 2007) |
| Benzoic acid | 1.9 | EPI Suite Database(EPA 2007) |
| Benzyl alcohol | 1.1 | EPI Suite Database(EPA 2007) |
| Bis(2-chloroethoxy) methane | 1.3 | McFarland (1995) |
| Carbazole | 3.2 | EPI Suite Database (EPA 2007) |
| Dibenzofuran | 3.7 | EPI Suite Database (EPA 2007) |
| Hexachlorobenzene | 5.2 | McFarland (1995) |
| Hexachlorobutadiene | 4.7 | EPI Suite Database (EPA 2007) |
| Hexachloroethane | 4.0 | EPI Suite Database (EPA 2007) |
| Nitrobenzene | 1.8 | EPI Suite Database (EPA 2007) |
| N-Nitrosodiphenylamine | 3.1 | McFarland (1995) |
| **Phthalates** | | |
| Bis(2-ethylhexyl) phthalate | 4.2 | McFarland (1995) |
| Butylbenzyl phthalate | 4.4 | EPA (1994) |
| Dibutyl phthalate | 4.6 | EPI Suite Database (EPA 2007) |
| Diethyl phthalate | 2.7 | EPI Suite Database (EPA 2007) |
| Dimethyl phthalate | 1.6 | McFarland (1995) |
| **Phenols** | | |
| 2-Methylphenol | 2.1 | EPI Suite Database (EPA 2007) |
| 4-Methylphenol | 2.1 | EPI Suite Database (EPA 2007) |
| 4-Nitrophenol | 1.9 | EPI Suite Database (EPA 2007) |
| Pentachlorophenol | 5.0 | McFarland (1995) |
| Phenol | 1.5 | McFarland (1995) |
| **PCBs** | | |
| Aroclor 1248 | 6.2 | EPA (1994) |
| Aroclor 1260 | 6.9 | McFarland (1995) |
| PCB 1 | 4.5 | Hawker & Connell (1988) |
| PCB 2 | 4.7 | Hawker & Connell (1988) |
| PCB 3 | 4.7 | Hawker & Connell (1988) |
| PCB 4 | 4.7 | Hawker & Connell (1988) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| PCB 5 | 5.0 | Hawker & Connell (1988) |
| PCB 6 | 5.1 | Hawker & Connell (1988) |
| PCB 7 | 5.1 | Hawker & Connell (1988) |
| PCB 8 | 5.1 | Hawker & Connell (1988) |
| PCB 9 | 5.1 | Hawker & Connell (1988) |
| PCB 10 | 4.8 | Hawker & Connell (1988) |
| PCB 11 | 5.3 | Hawker & Connell (1988) |
| PCB 12 & 13 | 5.3[b] | Hawker & Connell (1988) |
| PCB 14 | 5.3 | Hawker & Connell (1988) |
| PCB 15 | 5.3 | Hawker & Connell (1988) |
| PCB 16 | 5.2 | Hawker & Connell (1988) |
| PCB 17 | 5.3 | Hawker & Connell (1988) |
| PCB 18 | 5.2 | Hawker & Connell (1988) |
| PCB 18 & 30 | 5.3[b] | Hawker & Connell (1988) |
| PCB 19 | 5.0 | Hawker & Connell (1988) |
| PCB 20 & 28 | 5.6[b] | Hawker & Connell (1988) |
| PCB 21 & 33 | 5.6[b] | Hawker & Connell (1988) |
| PCB 22 | 5.6 | Hawker & Connell (1988) |
| PCB 23 | 5.6 | Hawker & Connell (1988) |
| PCB 24 | 5.4 | Hawker & Connell (1988) |
| PCB 25 | 5.7 | Hawker & Connell (1988) |
| PCB 26 & 29 | 5.6[b] | Hawker & Connell (1988) |
| PCB 27 | 5.4 | Hawker & Connell (1988) |
| PCB 28 | 5.7 | Hawker & Connell (1988) |
| PCB 31 | 5.7 | Hawker & Connell (1988) |
| PCB 32 | 5.4 | Hawker & Connell (1988) |
| PCB 33 | 5.6 | Hawker & Connell (1988) |
| PCB 34 | 5.7 | Hawker & Connell (1988) |
| PCB 35 | 5.8 | Hawker & Connell (1988) |
| PCB 36 | 5.9 | Hawker & Connell (1988) |
| PCB 37 | 5.8 | Hawker & Connell (1988) |
| PCB 38 | 5.8 | Hawker & Connell (1988) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| PCB 39 | 5.9 | Hawker & Connell (1988) |
| PCB 40 & 41 & 71 | 5.8[b] | Hawker & Connell (1988) |
| PCB 42 | 5.8 | Hawker & Connell (1988) |
| PCB 43 | 5.8 | Hawker & Connell (1988) |
| PCB 44 | 5.8 | Hawker & Connell (1988) |
| PCB 44 & 47 & 65 | 5.8[b] | Hawker & Connell (1988) |
| PCB 45 & 51 | 5.6[b] | Hawker & Connell (1988) |
| PCB 46 | 5.5 | Hawker & Connell (1988) |
| PCB 48 | 5.8 | Hawker & Connell (1988) |
| PCB 49 | 5.9 | Hawker & Connell (1988) |
| PCB 49 & 69 | 5.9[b] | Hawker & Connell (1988) |
| PCB 50 & 53 | 5.6[b] | Hawker & Connell (1988) |
| PCB 52 | 5.8 | Hawker & Connell (1988) |
| PCB 54 | 5.2 | Hawker & Connell (1988) |
| PCB 55 | 6.1 | Hawker & Connell (1988) |
| PCB 56 | 6.1 | Hawker & Connell (1988) |
| PCB 57 | 6.2 | Hawker & Connell (1988) |
| PCB 58 | 6.2 | Hawker & Connell (1988) |
| PCB 59 & 62 & 75 | 6.0[b] | Hawker & Connell (1988) |
| PCB 60 | 6.1 | Hawker & Connell (1988) |
| PCB 61 & 70 & 74 & 76 | 6.1[b] | Hawker & Connell (1988) |
| PCB 63 | 6.2 | Hawker & Connell (1988) |
| PCB 64 | 6.0 | Hawker & Connell (1988) |
| PCB 66 | 6.2 | Hawker & Connell (1988) |
| PCB 67 | 6.2 | Hawker & Connell (1988) |
| PCB 68 | 6.3 | Hawker & Connell (1988) |
| PCB 70 | 6.2 | Hawker & Connell (1988) |
| PCB 72 | 6.3 | Hawker & Connell (1988) |
| PCB 73 | 6.0 | Hawker & Connell (1988) |
| PCB 74 | 6.2 | Hawker & Connell (1988) |
| PCB 77 | 6.4 | Hawker & Connell (1988) |
| PCB 78 | 6.4 | Hawker & Connell (1988) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| PCB 79 | 6.4 | Hawker & Connell (1988) |
| PCB 80 | 6.5 | Hawker & Connell (1988) |
| PCB 81 | 6.4 | Hawker & Connell (1988) |
| PCB 82 | 6.2 | Hawker & Connell (1988) |
| PCB 83 & 99 | 6.3[b] | Hawker & Connell (1988) |
| PCB 84 | 6.0 | Hawker & Connell (1988) |
| PCB 85 & 116 & 117 | 6.4[b] | Hawker & Connell (1988) |
| PCB 86 & 87 & 97 & 108 & 119 & 125 | 6.4[b] | Hawker & Connell (1988) |
| PCB 87 | 6.3 | Hawker & Connell (1988) |
| PCB 88 & 91 | 6.1 | Hawker & Connell (1988) |
| PCB 89 | 6.1 | Hawker & Connell (1988) |
| PCB 90 | 6.4 | Hawker & Connell (1988) |
| PCB 090 & 101 & 113 | 6.4[b] | Hawker & Connell (1988) |
| PCB 92 | 6.4 | Hawker & Connell (1988) |
| PCB 03 & 95 & 98 & 100 & 102 | 6.1[b] | Hawker & Connell (1988) |
| PCB 94 | 6.1 | Hawker & Connell (1988) |
| PCB 95 | 6.1 | Hawker & Connell (1988) |
| PCB 96 | 5.7 | Hawker & Connell (1988) |
| PCB 97 | 6.3 | Hawker & Connell (1988) |
| PCB 99 | 6.4 | Hawker & Connell (1988) |
| PCB 101 | 6.4 | Hawker & Connell (1988) |
| PCB 103 | 6.2 | Hawker & Connell (1988) |
| PCB 104 | 5.8 | Hawker & Connell (1988) |
| PCB 105 | 6.7 | Hawker & Connell (1988) |
| PCB 106 | 6.6 | Hawker & Connell (1988) |
| PCB 107 & 124 | 6.7[b] | Hawker & Connell (1988) |
| PCB 109 | 6.5 | Hawker & Connell (1988) |
| PCB 110 | 6.5 | Hawker & Connell (1988) |
| PCB 110 & 115 | 6.5[b] | Hawker & Connell (1988) |
| PCB 111 | 6.8 | Hawker & Connell (1988) |
| PCB 112 | 6.5 | Hawker & Connell (1988) |
| PCB 114 | 6.7 | Hawker & Connell (1988) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| PCB 118 | 6.7 | Hawker & Connell (1988) |
| PCB 119 | 6.6 | Hawker & Connell (1988) |
| PCB 120 | 6.8 | Hawker & Connell (1988) |
| PCB 121 | 6.6 | Hawker & Connell (1988) |
| PCB 122 | 6.6 | Hawker & Connell (1988) |
| PCB 123 | 6.7 | Hawker & Connell (1988) |
| PCB 126 | 6.9 | Hawker & Connell (1988) |
| PCB 127 | 7.0 | Hawker & Connell (1988) |
| PCB 128 | 6.7 | Hawker & Connell (1988) |
| PCB 128 & 166 | 6.8[b] | Hawker & Connell (1988) |
| PCB 129 & 138 & 160 & 163 | 6.9[b] | Hawker & Connell (1988) |
| PCB 130 | 6.8 | Hawker & Connell (1988) |
| PCB 131 | 6.6 | Hawker & Connell (1988) |
| PCB 132 | 6.6 | Hawker & Connell (1988) |
| PCB 133 | 6.9 | Hawker & Connell (1988) |
| PCB 134 & 143 | 6.6[b] | Hawker & Connell (1988) |
| PCB 135 & 151 & 154 | 6.7[b] | Hawker & Connell (1988) |
| PCB 136 | 6.2 | Hawker & Connell (1988) |
| PCB 137 | 6.8 | Hawker & Connell (1988) |
| PCB 138 | 6.8 | Hawker & Connell (1988) |
| PCB 139 & 140 | 6.7[b] | Hawker & Connell (1988) |
| PCB 141 | 6.8 | Hawker & Connell (1988) |
| PCB 142 | 6.5 | Hawker & Connell (1988) |
| PCB 144 | 6.7 | Hawker & Connell (1988) |
| PCB 145 | 6.3 | Hawker & Connell (1988) |
| PCB 146 | 6.9 | Hawker & Connell (1988) |
| PCB 147 & 149 | 6.7[b] | Hawker & Connell (1988) |
| PCB 148 | 6.7 | Hawker & Connell (1988) |
| PCB 149 | 6.7 | Hawker & Connell (1988) |
| PCB 150 | 6.3 | Hawker & Connell (1988) |
| PCB 151 | 6.6 | Hawker & Connell (1988) |
| PCB 152 | 6.2 | Hawker & Connell (1988) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| PCB 153 | 6.9 | Hawker & Connell (1988) |
| PCB 153 & 168 | 7.0[b] | Hawker & Connell (1988) |
| PCB 155 | 6.4 | Hawker & Connell (1988) |
| PCB 156 | 7.2 | Hawker & Connell (1988) |
| PCB 156 & 157 | 7.2[b] | Hawker & Connell (1988) |
| PCB 157 | 7.2 | Hawker & Connell (1988) |
| PCB 158 | 7.0 | Hawker & Connell (1988) |
| PCB 159 | 7.2 | Hawker & Connell (1988) |
| PCB 161 | 7.1 | Hawker & Connell (1988) |
| PCB 162 | 7.2 | Hawker & Connell (1988) |
| PCB 164 | 7.0 | Hawker & Connell (1988) |
| PCB 165 | 7.1 | Hawker & Connell (1988) |
| PCB 166 | 6.9 | Hawker & Connell (1988) |
| PCB 167 | 7.3 | Hawker & Connell (1988) |
| PCB 168 | 7.1 | Hawker & Connell (1988) |
| PCB 169 | 7.4 | Hawker & Connell (1988) |
| PCB 170 | 7.3 | Hawker & Connell (1988) |
| PCB 171 & 173 | 7.1[b] | Hawker & Connell (1988) |
| PCB 172 | 7.3 | Hawker & Connell (1988) |
| PCB 174 | 7.1 | Hawker & Connell (1988) |
| PCB 175 | 7.2 | Hawker & Connell (1988) |
| PCB 176 | 6.8 | Hawker & Connell (1988) |
| PCB 177 | 7.1 | Hawker & Connell (1988) |
| PCB 178 | 7.1 | Hawker & Connell (1988) |
| PCB 179 | 6.7 | Hawker & Connell (1988) |
| PCB 180 | 7.4 | Hawker & Connell (1988) |
| PCB 180 & 193 | 7.4[b] | Hawker & Connell (1988) |
| PCB 181 | 7.1 | Hawker & Connell (1988) |
| PCB 182 | 7.2 | Hawker & Connell (1988) |
| PCB 183 | 7.2 | Hawker & Connell (1988) |
| PCB 183 & 185 | 7.2[b] | Hawker & Connell (1988) |
| PCB 184 | 6.9 | Hawker & Connell (1988) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| PCB 186 | 6.7 | Hawker & Connell (1988) |
| PCB 187 | 7.2 | Hawker & Connell (1988) |
| PCB 188 | 6.8 | Hawker & Connell (1988) |
| PCB 189 | 7.7 | Hawker & Connell (1988) |
| PCB 190 | 7.5 | Hawker & Connell (1988) |
| PCB 191 | 7.6 | Hawker & Connell (1988) |
| PCB 192 | 7.5 | Hawker & Connell (1988) |
| PCB 194 | 7.8 | Hawker & Connell (1988) |
| PCB 195 | 7.6 | Hawker & Connell (1988) |
| PCB 196 | 7.7 | Hawker & Connell (1988) |
| PCB 197 & 200 | 7.3[b] | Hawker & Connell (1988) |
| PCB 198 & 199 | 7.4[b] | Hawker & Connell (1988) |
| PCB 201 | 7.6 | Hawker & Connell (1988) |
| PCB 202 | 7.2 | Hawker & Connell (1988) |
| PCB 203 | 7.7 | Hawker & Connell (1988) |
| PCB 204 | 7.3 | Hawker & Connell (1988) |
| PCB 205 | 8.0 | Hawker & Connell (1988) |
| PCB 206 | 8.1 | Hawker & Connell (1988) |
| PCB 207 | 7.7 | Hawker & Connell (1988) |
| PCB 208 | 7.7 | Hawker & Connell (1988) |
| PCB 209 | 8.2 | Hawker & Connell (1988) |
| **Dioxins and furans** | | |
| 2,3,7,8-Tetrachlorodibenzofuran | 6.3 | EPI Suite Database (EPA 2007) |
| 2,3,7,8-Tetrachlorodibenzo-*p*-dioxin | 6.9 | EPI Suite Database (EPA 2007) |
| 2,3,4,6,7,8-Hexachlorodibenzofuran | 7.6 | EPI Suite Database (EPA 2007) |
| 2,3,4,7,8-Pentachlorodibenzofuran | 6.9 | EPI Suite Database (EPA 2007) |
| 1,2,3,4,6,7,8-Heptachlorodibenzofuran | 8.2 | EPI Suite Database (EPA 2007) |
| 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin | 8.8 | EPI Suite Database (EPA 2007) |
| 1,2,3,4,7,8,9-Heptachlorodibenzofuran | 8.2 | EPI Suite Database (EPA 2007) |
| 1,2,3,4,7,8-Hexachlorodibenzofuran | 7.6 | EPI Suite Database (EPA 2007) |
| 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin | 8.2 | EPI Suite Database (EPA 2007) |
| 1,2,3,6,7,8-Hexachlorodibenzofuran | 7.6 | EPI Suite Database (EPA 2007) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin | 8.2 | EPI Suite Database (EPA 2007) |
| 1,2,3,7,8,9-Hexachlorodibenzofuran | 7.6 | EPI Suite Database (EPA 2007) |
| 1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin | 8.2 | EPI Suite Database (EPA 2007) |
| 1,2,3,7,8-Pentachlorodibenzofuran | 6.9 | EPI Suite Database (EPA 2007) |
| 1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin | 7.6 | EPI Suite Database (EPA 2007) |
| Octachlorodibenzofuran | 8.9 | EPI Suite Database (EPA 2007) |
| Octachlorodibenzo-*p*-dioxin | 9.5 | EPI Suite Database (EPA 2007) |
| **Pesticides** | | |
| 2,4-DDD | 5.9 | Howard & Meylan (1997) |
| 2,4-DDE | 6.0 | Howard & Meylan (1997) |
| 2,4-DDT | 6.8 | Howard & Meylan (1997) |
| 4,4-DDD | 6.0 | Howard & Meylan (1997) |
| 4,4-DDE | 6.5 | Howard & Meylan (1997) |
| 4,4-DDT | 6.9 | Howard & Meylan (1997) |
| Aldrin | 6.8 | EPI Suite Database (EPA 2007) |
| alpha-Endosulfan | 3.6 | McFarland (1995) |
| alpha-Hexachlorocyclohexane | 3.8 | McFarland (1995) |
| beta-Endosulfan | 3.6 | McFarland (1995) |
| beta-Hexachlorocyclohexane | 3.8 | McFarland (1995) |
| cis-Chlordane | 6.3 | EPI Suite Database (EPA 2007) |
| cis-Nonachlor | 6.4 | EPI Suite Database (EPA 2007) |
| delta-Hexachlorocyclohexane | 3.8 | McFarland (1995) |
| Dieldrin | 5.5 | McFarland (1995) |
| Endosulfan sulfate | 3.6 | McFarland (1995) |
| Endrin | 4.6 | McFarland (1995) |
| Endrin aldehyde | 5.6 | McFarland (1995) |
| Endrin ketone | 5.0 | EPI Suite Database (EPA 2007) |
| gamma-Hexachlorocyclohexane | 3.8 | McFarland (1995) |
| Heptachlor | 5.4 | McFarland (1995) |
| Heptachlor epoxide | 4.6 | EPI Suite Database (EPA 2007) |
| Methoxychlor | 4.3 | McFarland (1995) |
| Oxychlordane | 5.5 | EPI Suite Database (EPA 2007) |

**Table 5-1. $K_{ow}$s for Neutral Organic Chemicals**

| COI | log $K_{ow}$ | Source |
|---|---|---|
| trans-Chlordane | 6.3 | EPI Suite Database (EPA 2007) |
| trans-Nonachlor | 6.4 | EPI Suite Database (EPA 2007) |

[a] Kow based on average Kow reported in multiple sources.

[b] For PCB congener coelutions, the average of the log $K_{ow}$ of the coeluting chemicals was used for the coelution.

COI – chemical of interest

EPA – US Environmental Protection Agency

PAH – polycyclic aromatic hydrocarbon

PCB – polychlorinated biphenyl

SVOC – semivolatile organic compound

# 6.0 SIGNIFICANT FIGURES

The laboratory reported results with different numbers of significant figures depending on the instrument, parameter, and the concentration relative to the DL. 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 when totaling PCBs or PAHs, the calculation could 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 involved multiplication or division, such as when carbon normalizing was used, all significant figures were carried through the calculation, and then the total result was 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 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.

Analytical results are reported as they appeared in the SCRA database. Significant figures were not explicitly tracked in the SCRA database, therefore a result of 1.0, which has two significant figures, appeared to have only one when the significant figures were identified as non-zero integers. A minimum of two significant figures was used for all results. This is consistent with the standard reporting requirements of analytical laboratories. This step was necessary to ensure that summary calculations were not forced to one significant figure because of trailing zeros.

# 7.0 FIELD REPLICATES

This section presents the data management rules for the treatment of field replicates (Section 7.1). A field replicate is a separate sample collected at approximately the same location and is intended to be a measure of environmental variability for the parameters or analytes being measured.

## 7.1 FIELD REPLICATES

Field replicates were treated as independent samples during data analysis. In geographic information system (GIS) applications, such as the calculation of spatially weighted average concentrations (SWACs), the calculation requires one result for each coordinate location. A small subset of surface sediment field replicates had coordinates identical to those of the parent samples. Data associated with the first sample was used for replicates that have the same coordinates (the second or third replicate is excluded). Replicates with unique coordinates were included as separate samples. Surface sediment field replicates excluded from GIS exports to prevent mapping errors are presented in Table 7-1.

Table 7-1. Surface Sediment Field Replicates Excluded from GIS Exports

| Sample Type | Sample ID |
|---|---|
| LWG field replicates | LW2-B022-2 |
| | LW2-B025-2 |
| | LWG0109B027SDS015C20 |
| | LWG0109B027SDS015C31 |
| | LW2-GBT006-2 |
| | LW2-GBT027-2 |
| Non-LWG field replicates | PSYSEA98PSY08PSY52S |
| | PSYSEA98PSY08PSY53S |
| | PSYSEA98PSY72PSY74S |
| | PSYSEA98PSY72PSY75S |
| | WLCGSD01AN0101_10-20 |
| | WLCGSD01AN0102_10-20 |
| | WLCGSD01AN0103_10-20 |
| | WLCGSD01AN0105_10-20 |
| | WLCGSD01AN0205_10-20 |
| | WLCASF97S012W4169 |
| | WLCASF97S045W4162 |
| | WLCDRD05PG141141Dup |
| | WLCDRD05PG140140Dup |
| | WLCDRD05PG137137Dup |

Table 7-1. Surface Sediment Field Replicates Excluded from GIS Exports

| Sample Type | Sample ID |
|---|---|
| | WLCDRD05PG139139Dup |
| | WLCDRD05PG136136Dup |
| | WLCDRD05PG135135Dup |
| | WLCDRD05PG138138Dup |

GIS – geographic information system
ID – identification

# 8.0 SURFACE WATER DATA COLLECTED BY DIFFERENT METHODS

This section presents the data management rules for the representation of surface water data collected using XAD filters, XAD columns, and peristaltic pump. The surface water XAD column and XAD filter data were combined for comparison to criteria based on totals using the following rules:

- If both XAD results were detected, the two values were summed.
- If one XAD result was not detected and the other result was detected, the detected value was used.
- If both XAD results were not detected, the maximum DL was used.

The XAD samples and the peristaltic samples were treated as separate samples.

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