Description of Procedures for Calculating PCB Sums in NOAA DIVER Regional Databases

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Background Information

The DIVER Data Warehouse[1] contains nearly 30 years of NOAA data management of environmental data, with continuity from the legacy Query Manager (QM) data management system. The following summary describes the overall approach for standardizing, calculating and managing Sums (Totals) for PCBs (Polychlorinated Biphenyls) in the DIVER Data Warehouse for Samples data which includes sediment, tissue and water matrices. In addition to this overarching summary, it is important for data users to review the Study Notes which are associated with each Study in DIVER. These Study Notes were generated with the original data standardization and integration effort beginning in Query Manager from the mid 1990's - early 2010s, and have been updated where appropriate and continue to be generated for environmental data added to DIVER. Two key fields in the DIVER Samples Data Category[2] are the Chemcode field, and the Analysis (or Chemical Name) field. The following explanations provides details referencing the Chemcode field (e.g., PCB_SUM_A) and the Analysis text (e.g., "PCBs, total Aroclors (QM calculated)")

PCB Sums Calculated By The Data Management Team

PCB_SUM_A "PCBs, total Aroclors (QM calculated[3])"	**PCB_SUM_A** is the calculated sum of Aroclors. At least 2 Aroclors must be present to report a calculated Aroclor sum.
PCB_SUM_P "PCBs, total congeners (QM calculated)"	**PCB_SUM_P** is the calculated sum of PCB congeners. There are 209 potential single compound congeners as well as numerous co-elution combinations. In general, PCB_SUM_P is appended to the database if there are 30 or more reported congener records. However, there are studies (e.g., NOAA Status and Trends Mussel Watch, EMAP, etc.) where an investigator may have used the NOAA Status and Trends (NST) approach to estimating Total PCB based on a subset of 18 congeners or 18 congeners plus the set of coplanar congeners. Where there are 17 or more congeners, but fewer than 30 congeners, the total PCB result is based on the sum of the list of NS&T 18 congeners multiplied by 2. The method of PCB congener summing used is noted in the Study Notes.
PCB_SUM_H "PCBs, total homologs (QM calculated)"	**PCB_SUM_H** is the calculated sum of PCB homologs (e.g., PCBS_CL1… PCBS_CL10, sum of monochloro biphenyl congeners through the decachloro biphenyl congeners). These sums are only appended if 9 or 10 of the homologs are included in the sum. The number of analytes included in sums is shown in the QAULCODE field.

[1] Public DIVER website: https://www.diver.orr.noaa.gov
[2] Detailed information in the DIVER Data Specification found here: https://diver.orr.noaa.gov/web/guest/data-overview
[3] We continue to use "QM calculated" in terminology to highlight continuity with past calculation and summation processes

PCB Sums Reported In Source Data

PCB_SUMR “PCBs, total (reported)”
PCB_SUM_AR “PCBs, total Aroclors (reported)”
PCB_SUM_HR “PCBs, total homologs (reported)”
PCB_SUM_PR “PCBs, total congeners (reported)”

Reported sums given with the original data submission are coded as PCB_SUM_AR (reported Aroclor sum), PCB_SUM_HR (reported homolog sum) or PCB_SUM_PR (reported congener sum). If the type of reported sum is not stated but the information is available, the type can be determined by a review of the values and other analytes reported in the data set. For example, when the study only reported Aroclors and there is no mention of other individual congener analysis, a “reported Aroclor sum” can be assigned to the record. Any known information regarding the derivation of the reported sum (for example handling of non-detects as zero or at half the detection limit) is recorded in the Study Notes. In rare cases where there is a PCB sum reported without any of the individual analytes and it is not possible from the material to determine whether it is a congener or Aroclor sum, then the result is reported as PCB_SUMR. These are the most common reported sums. Additional regional or project-specific sums, such as using the NOAA 1989 method (PCB_SUM_C “PCBs, total congeners (NOAA 1989)”) or the total of all co-planar congeners (PCB_SUMLR “PCBs, total co-planar (reported)”), may also be reported and will be described in the Study notes.

Primary PCB sum assignment

PCB_SUM “PCBs, total (QM calculated)”

Once all the calculated PCBs have been derived, a sum that will be recorded as the “primary” PCB sum for each study is determined. The purpose of having a primary or chosen PCB_SUM value was originally for use in queries that compare values to guidelines (e.g. sediment or tissue). The choice of primary PCB sum is study specific and is documented in the Study Notes for every study. The preferred choice usually is the calculated PCB_SUM_P from congeners if these sums are available for all samples. However, if there are more samples that were analyzed for Aroclors than were analyzed for PCB congeners, then the Aroclor sum is preferred because it was analyzed in more of the samples. In some circumstances, the NOAA case team responsible for the site will request that a calculated Aroclor sum or reported sum is used for PCB_SUM for specific studies regardless of other sums that might be available. For example, Hudson River sediment samples use the calculated Aroclor sum as the primary PCB_SUM while fish tissue samples use the reported Aroclor sum as the primary PCB_SUM value due to long standing case team preference.

Qualifier Codes (QUALCODE)

When sums are calculated in the DIVER Data Warehouse, the QUALCODE field is generally filled in with details on how many analytes were reported and not rejected, and how many were “U” qualified (below the method detection limit). Specific details are in each Study’s “Study Notes” file, however the procedure and notation are typically uniform. Where analytes were available for a sum from a specific list of analytes, sums are recalculated and qualified with ‘CALC’ or ‘UCALC’ followed by a number representing the total number of analytes reported and not rejected (e.g., ‘CALC_008’). In the summing procedure, non-detected compounds are treated as zeros (rejected results are excluded). If all compounds that comprise the total were not detected or the detection limit of any one non-detect compounds is greater than the sum, then the highest non-detect value is reported with a ‘UCALC’ qualifier (e.g., UCALC_008)

More Information

DIVER Data Specification including Chemical Codes and Chemical Names

Reference information on PCB Congeners (EPA)

2023-2024 DIVER Updates to PCB Congener and Aroclor Naming Conventions

The original DIVER data dictionary utilized the Ballschmiter-Zell (BZ) system for PCB congener numbering with a database chemcode starting with the prefix “PCB” and the dictionary chemical name starting with the prefix “BZ#”. However, as the database expanded, the same BZ labeling format was not applied in the same manner to all additions of new PCB congener analytes when the PCB congeners were reported as co-eluting mixtures. To increase the readability and consistency of the PCB congener chemical names as they appear in DIVER, the following updates to the dictionary chemical name text were implemented across all DIVER regional databases:

- Replaced the code “BZ#” with “PCB” in analyte names.
- Removed redundant phrases of “co-elution of” and “congener” from analyte names and removed unnecessary chlorination group labels (like “Cl4”) for co-eluting congener mixes.
- Used ampersands (&) for multiple co-eluting congeners and made lists be separated by spaces. Thus, chemical names with dashes, slashes, and plus signs were updated.
- A zero was added to two-digit congener numbers so all congeners have three-digit numbers.
- Spaces between PCB label and congener numbers were removed and lists of congeners were updated to have only one PCB suffix at the beginning of the list.
- Incomplete 13C12 labels were repaired for radiolabeled PCB congeners, which designates a 13C-labeled congener.
- The name Aroclor was spelled out when it was present as the abbreviation “Ar”
- Note that the phrase “revised code” was kept when present in previous chemical names.

Example Study Notes Text

GE Fish Tissue data, 2005 [W2]

DATA SOURCE

Original data came from EPA_Export.mdb within GE061215_Export_Fish.zip. On 2/2/2016, added results for 32 laboratory replicates from EPA_Export_Fish_2015-01-29.zip

DATA TYPES

This study includes results for tissue chemistry.

STATIONS

Original coordinates were in easting/northing in NY state plane NAD83 and were converted to latitude/longitude. Notes regarding converted coordinates: Locations represent generalized catch locations. NYSP coordinate start and stop locations were used to create electro-shocking catch trackline ArcView shapefiles. Shapefile projected to geographic coordinates using ArcView 3.3. Centroids created via Avenue scripts. Tracklines centroids manually edited/moved to appropriate in-river location where necessary (centroids falling on land). Tracklines centroid coordinates added in DD NAD83. StationIDs of TD5 and SW5 were changed to TD5S (spring), TD5F (fall), SW5S (spring), and SW5F (fall).

SAMPLES AND REPLICATES

Stationid is the first 3 digits of the Field id. Sampleid is the last 5-8 digits (describing species code and ID number). i.e. field id = AT1-040608-01-CHC-01 became station AT1 and sample CHC-01. Assigned labrep “b” to pcb sum from congeners (method NE013_07) as this was the least frequent PCB sum reported. Congener results associated with these PCB sums were also coded with labrep b. Sample length was converted from mm to cm by dividing by 10. Weight is reported in grams. Weight (total of all organisms) and length (average of all organisms) for composites were calculated from reported total weight and length.

CALCULATED RESULTS

=== General Summing Conventions === Where the source data included sums, these values were maintained and coded with a CHEMCODE/Chemical name that indicated these are “reported” results (see specifics below). Where the appropriate analytes were available, sums were recalculated and qualified with ‘CALC’ or ‘UCALC’ followed by a number representing the total number of analytes reported and not rejected (e.g., ‘CALC_008’). In the summing procedure, non-detected compounds are treated as zeros (rejected results are excluded). If all compounds that comprise the total were not detected or the detection limit of any one non-detect compounds is greater than the sum, then the highest non-detect value is reported with a ‘UCALC’ qualifier (e.g., UCALC_008). Details regarding the specific compounds included in the sums are provided in the paragraphs below. === Grain Size === === PAH Sums === === PCB Sums === The original reported PCB sums from the source data were assigned the chemcode PCB_SUM. Those from Aroclor analysis have a Labrep = 1 or 2. Those from congener analysis have a Labrep = b or b2. The records for PCB_SUM were copied and assigned either Chemcode PCB_SUM_AR (for Aroclor sums) or PCB_SUM_PR (for congener sums) as appropriate. Total PCBs from congener data were calculated and reported with a CHEMCODE = PCB_SUM_P. Total PCBs from Aroclor data were calculated and reported with a CHEMCODE = PCB_SUM_A. === DDT Sums === === Chlordane Sums === === Simultaneously Extracted Metals ===

QUALIFIERS

No qualifiers descriptions were provided. Assumptions were made that U = undetected and J = estimated. Description of qualifier =” * “ is unknown.

Lower Duwamish Sediment Sampling 2020 [V1]

DATA SOURCE

Source: NOAA

STUDY PURPOSE

This study was conducted as part of the Lower Duwamish River natural resource damage assessment. The purpose was to collect surficial sediment samples near Harbor Island and upstream for chemical analysis of PAHs, PCBs, and metals, with an overarching objective to evaluate the nature, magnitude, and extent of sediment contamination within the LDR assessment area and upstream. Sediment samples were collected in October 2020 and sent to Axys and ALS for chemical analysis. The data were then validated by EcoChem at Level 2B or better.

DATA USE QUALIFICATION

The data validation indicated on the source data was EPA Stage 2B, EPA Stage 3, and EPA Stage 4. The validator is EcoChem, Inc. This description has been standardized to VALSUMM (summary validation) in the DVLevel field of the chemistry tables. Data from the ALS laboratory have the method detection limit (MDL) in the ”Detection Limit” field and the reporting limit in the ”Reporting Limit” field for most analytes. For alkylated PAHs, the detection limit is given the same value as the reporting limit, because the lab only determines MDLs for the parent PAHs. Data from the Axys laboratory have the method detection limit in the ”Detection Limit” field determined as specified by EPA Fed. Reg. 40 CFR Part 136 Appendix B (Rev.1 or Rev.2, as documented for each method/matrix). MDL is determined as required based on accreditation, contract and workload requirements. The MDL determination is a general demonstration of method detection limit. It is performed at a particular time, using a set of sample prepared using clean matrix, and may not account for all matrix effects encountered in environmental samples. Data from the Axys laboratory have the sample-specific detection limit (SDL) in the ”Reporting Limit” field determined by converting the area equivalent of 3.0 times (2.5 times for EPA 1600 series methods) the estimated chromatographic noise height to a concentration in the same manner that target peak responses are converted to final concentrations. Determined individually for every sample analysis run. The SDL accounts for any effect of matrix on the detection system and for recovery achieved through the analytical work-up. It does not account for any lab background input.

DATA TYPES

This study includes results for surficial sediment.

STATIONS

Station identifiers were included as they were presented in the source data without modification. The original coordinates were provided in the WGS84 datum. Coordinates were converted to NAD83 latitude and longitude using QGIS. The original coordinates were plotted using WGS84 and converted to a shapefile in QGIS. QGIS tools were used to re-define the projection to Geographic Coordinate System to NAD83.

SAMPLES AND REPLICATES

The Sample identifiers reported in the source data are stored in the ExSampID field. Sampling dates and sample depth information were provided for all samples.

CHEMISTRY

Rejected results are included in the database and not modified; the associated QUALCODE includes R. The sums of the grainsize fractions exceed 100% in the source data and were incuded as is. In the source file, chemical concentrations for co-eluting PCB congeners were reported as two separate records, and flagged with a C qualifier code. These results were merged into one record, as per the database convention.

CALCULATED RESULTS

=== General Summing Conventions === Where the source data included sums, these values were maintained and coded with a CHEMCODE/Chemical name that indicated these are “reported” results (see specifics below). Where the appropriate analytes were available, sums were recalculated and qualified with ‘CALC’ or ‘UCALC’ followed by a number representing the total number of analytes reported and not rejected (e.g., ‘CALC_008’). In the summing procedure, non-detected compounds are treated as zeros (rejected results are excluded). If all compounds that comprise the total were not detected or the detection limit of any one non-detect compounds is greater than the sum, then the highest non-detect value is reported with a ‘UCALC’ qualifier (e.g., UCALC_008). Details regarding the specific compounds included in the sums are provided in the paragraphs below. === Grain Size === Results for %silt and %clay were summed to generate records for the chemcode = PCT_FINES. A sum is only calculated if there are two or more results for %silt and/or %clay. === PAH Sums === Total low molecular weight PAHs (chemcode = LPAH) were calculated for samples with two or more of the following chemicals reported: acenaphthene anthracene biphenyl 2,6-dimethylnaphthalene fluorene 1-methylnaphthene 2-methylnapthene 1-methylphenanthrene phenanthrene naphthalene CHEMCODES = ACENAPTHEN, ANTHRACENE, BIPHENYL, METNAP26_2, FLUORENE, METHNAP_1, METHNAP_2, METPHENAN1, PHENANTHRN, NAPTHALENE Total high molecular weight PAHs (chemcode = HPAH) were calculated for samples with two or more of the following chemicals reported: benz(a) anthracene benzo(a)pyrene benzo(e)pyrene chrysene dibenz(a,h)anthracene fluoranthene perylene pyrene CHEMCODES = BAA, BAP, BEP, CHRYSENE, BANTH2, FLUORANTHN, PERYLENE, PYRENE Total PAHs (chemcode = TOTAL_PAH) were calculated as the sum of the LPAH and HPAH chemicals as listed above. === PCB Sums === Total of PCB congeners were calculated and assigned the chemcode PCB_SUM_P. The total is the sum of congeners, with 30 or more congeners reported for each sample. Total PCB homologs were calculated and assigned the chemcode PCB_SUM_H for samples with nine or ten homologs reported. The congener sum was also reported with the chemcode PCB_SUM.

QUALIFIERS

Qualifiers definitions are provided in the qualifier table. Definitions were provided with the source data.