Using Qualified Data to Document an Observed Release and Observed Contamination

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This fact sheet discusses the use of the U.S. Environmental Protection Agency's (EPA) Contract Laboratory Program (CLP) data and other sources of data qualified with a "J", "U", or "UJ" qualifier or flag. This new fact sheet supersedes the existing 1996 fact sheet, Using Qualified Data to Document an Observed Release and Observed Contamination (OSWER 9285.7-14FS). This guidance provides a management decision tool for the optional use of qualified data to document observed release and observed contamination by chemical analysis under EPA's Hazard Ranking System (HRS)[1]. The analyte and sample matrix (i.e., soil or water) specific adjustment factors given in this fact sheet allow biased CLP and non-CLP data to be adjusted to meet the HRS criteria documenting an observed release and observed contamination with data that are of known and documented quality. Hereafter, throughout the fact sheet, "observed release" will generally refer to both observed release and observed contamination.[2]

INTRODUCTION

The EPA established the HRS to rank hazardous waste sites for National Priorities List purposes under the Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA) as amended by the Superfund Amendments and Reauthorization Act of 1986 (SARA). This fact sheet was developed in response to a need to determine the usability of qualified data for site assessment and HRS scoring purposes. This fact sheet illustrates that qualified data are often of sufficiently known and documented quality and may be used in establishing an observed release. This fact sheet explains the rationale for why some qualified data may be used for HRS purposes; presents the background information needed to use qualified data, with and without adjustment factors; provides examples of qualified data use; and discusses issues raised during the development of the adjustment factor approach.

Under the HRS, chemical analytical data are often used to demonstrate an observed release when the release sample concentration is three times the background concentration and background levels are greater than or equal to the appropriate detection limit; or if the release sample concentration is greater than or equal to the appropriate quantitation limit when background levels are below the appropriate detection limit. The release must also be at least partially attributable to the site under investigation (*Hazard Ranking System, Final Rule,* 40 CFR Part 300, App. A). The data used to establish the release must be of known and documented quality (*Hazard Ranking System Guidance Manual, Interim Final,* November 1992, OSWER Directive 9345.1-07). Data that cannot be validated may not be of known and documented quality. For more information on observed release and observed contamination, refer to the fact sheets: *Establishing an Observed Release,* September 1995; *Establishing Areas of Observed Contamination*. September 1995; and *Establishing Background Levels,* September 1995. The factor of three represents the minimum difference in sample results that demonstrate an increase in contaminant concentration above background levels, with reasonable confidence.

1 This fact sheet does not specifically address using qualified data for identifying hazardous substances in a source. However, in those situations where source samples may be compared to background to demonstrate the relative increase in source contaminant levels, the adjustment factors may be used.

2 This fact sheet currently addresses data used in documenting an observed release and observed contamination. While analyte-specific adjustment factors do not currently apply to gaseous/air sample results for the air migration pathway or subsurface intrusion component of the soil exposure and subsurface intrusion pathway, they can be applied to groundwater or soil sample results used in documenting an area of subsurface contamination. Analyte-specific adjustment factors for use with qualified gaseous/air sample results are under consideration.

Although much of the analytical data used for identifying an observed release is generated under CLP, this fact sheet applies to all data regardless of the source of the data (CLP data, non-CLP data). EPA procedures require that CLP analytical data be reviewed, or validated by EPA or third party reviewers, to ensure the data are of known and documented quality and that the determination be discussed in a data validation report that accompanies the analytical results. Based on this data validation, CLP data are classified into three general categories. First, data for which all quality control (QC) elements have passed contract required acceptance criteria are typically not qualified. Second, data for which at least one QC element has not met acceptance criteria are often qualified with a "J" qualifier indicating the reported results are estimates. Third, some data are rejected due to serious deficiencies in meeting QC requirements, are qualified "R", and are considered unusable for HRS purposes.

Whether data are placed into the second or third category is determined by the amount of bias associated with the analytical results. Data validation evaluates biases resulting from laboratory analytical deficiencies or sample matrices to determine whether the data are usable. Bias indicates that the reported concentration is either higher or lower than the true concentration, and the data validation report identifies the direction of the bias or if the bias is unknown.

The EPA CLP also sets minimum quantitation limits for all analytes, the Contract Required Quantitation Limit (CRQL). (For older CLP inorganic data, prior to 2004, this limit was referred to as the Contract Required Detection Limit [CRDL] and was equivalent to the CRQL.) The CRQLs are substance specific levels that a CLP laboratory must be able to routinely and reliably detect in specific sample matrices (i.e., soil, water, sediment). The CRQLs are usually set above most instrument detection limits (IDLs) and method detection limits (MDLs).

CONSIDERATIONS FOR NON-CLP DATA

Because various laboratories and analytical methods may be used to develop non-CLP data, the following list provides general information that may be useful in utilizing non-CLP data for HRS purposes.

(1) Identification of the method used for analysis. Methods may include SW-846 methods, EPA methods, etc.

(2) QC data. Each method of analysis may describe QC requirements specific to that method; associated QC data may be supplied with sample results documentation.

(3) Instrument-generated data sheets for sample results. These data sheets would be the equivalent of Form Is in CLP data.

(4) MDLs and sample quantitation limits (SQLs). Per the HRS, the MDL is the lowest concentration of an analyte that a method can detect reliably in either a sample or a blank. The analytical method may provide an MDL, or more often laboratories typically generate laboratory-specific MDLs. As a detection limit for real-time field instruments, the HRS also recognizes the detection limit of the instrument as used in the field. Per the HRS, the SQL represents the quantity of a substance that can be reasonably quantified given the limits of detection for the methods of analysis and sample characteristics that may affect quantitation (e.g., dilution, concentration, percent moisture content); it may be set either by the method, the laboratory at the lowest calibration point, or the laboratory as a multiple of the MDL.

(5) Data validation report.

USE OF BIASED QUALIFIED DATA

In the past, all qualified data may have been inappropriately perceived as data of low confidence or poor quality and had not been used in the earliest HRS evaluations. However, with careful assessment of the nature of the analytical biases or QC deficiencies in the data on a case-by-case basis, qualified data can represent an additional resource of data for establishing an observed release. Further, the U.S. Court of Appeals, D.C. Circuit in 1996 upheld EPA's case-by-case approach to assess data quality. In reviewing the quality of data used to identify an observed release, the Court concurred that if there are deficiencies in the data, "…the appropriate response is to review the deficiencies on a 'case-by-case basis' to determine their impact on 'the usability of the data.'" The Court also stated with regards to data quality that, "…EPA does not face a standard of absolute perfection…Rather, it is statutorily required to 'assure, to the maximum extent feasible,' that it 'accurately assesses the relative degree of risk' posed by sites" [*Board of Regents of the University of Washington, et al.,* v. EPA, No. 95-1324, slip op. at 8-10 (D.C. Cir. June 25, 1996).]

As discussed in this fact sheet, the application of adjustment factors to "J" qualified data can serve as a management decision tool to "adjust," or take into account, the analytical uncertainty in the data indicated by the qualifier, thereby making qualified data usable for an HRS evaluation. The use of adjustment factors to account for the larger uncertainty in "J" qualified data is a conservative approach enabling a quantitative comparison of the data for use in documenting an observed release. Some guidelines for using the adjustment factor approach are discussed in Exhibit 1.

EXHIBIT 1
GUIDELINES FOR THE USE OF ADJUSTMENT FACTORS

!	The use of adjustment factors identified in this fact sheet is a management tool for the optional use of "J" qualified data generated under CLP or other sources of data to document an observed release.
!	Adjustment of qualified data should be used with non-qualified data whenever possible.
!	EPA Regions should use adjustment factors with discretion on a case-by-case basis and should always carefully consider the use of qualified data in borderline cases.
!	EPA Regions may substitute higher adjustment factors based on documented, justifiable reasons but may never use a lower adjustment factor value.
!	The adjustment factors should only be applied to analytes listed in the tables. Although the adjustment factors were generated based primarily on data from samples analyzed by CLP methods, they can be applied to the same analytes analyzed by other similar methodologies. These adjustment factors should not be interpolated or extrapolated to develop factors for analytes not listed in the tables.
!	"UJ" data may be used without adjustment as explained in this fact sheet.
!	The adjustment factors only apply to biased "J" qualified data, not to other "J" qualified data such as results qualified "J" solely due to detection between the detection limit and quantitation limit.
!	The adjustment factors do not apply to "NJ" or "R" qualified data. These data cannot be used to document an observed release for HRS purposes.

CLP QA/QC PROCEDURES

CLP qualifiers are applied to analytical data based on the results of various Quality Assurance/Quality Control (QA/QC) procedures used at the laboratory. EPA analytical methods use a number of QA/QC mechanisms during sample analysis in order to assess qualitative and quantitative accuracy. (For example, see the CLP Statements of Work, EPA SW-846 Compendium methods, and CLP guidance for field samplers.[3]) To assess data quality, the laboratory uses various QC elements including matrix spikes, matrix spike duplicates, laboratory control samples, surrogates, blanks, laboratory duplicates, and quarterly blind performance evaluation (PE) samples. The Agency assumes that if biases are found in the QA/QC samples, the field sample concentrations may also be biased.

Surrogates are chemically similar to the analytes of interest. They are added or "spiked" at a known concentration into the field samples before analysis. Also, selected target analytes are "spiked" into samples at a specified frequency to assess potential interferences from the sample matrix. These samples are called matrix spikes. Comparison of the known concentration of the surrogates and matrix spikes with their actual analytical results reflects the analytical accuracy. Because the surrogates are expected to behave similarly to the target analytes, they may indicate bias caused by interferences from the sample matrices. These type of interferences from the sample matrix are known as matrix effects.[4]

Laboratory control samples are zero blind samples which contain known concentrations of specific analytes and are analyzed in the same batch as field samples. Their results are used to measure laboratory accuracy. Blanks are analyzed to detect any extraneous contamination introduced either in the field or in the laboratory.

Laboratory duplicates are created when one sample undergoes two separate analyses. The duplicate results are compared to determine laboratory precision. Quarterly blind PE samples are single blind samples that evaluate the laboratory's capability of performing the specified analytical protocol.

CLP and other EPA analytical methods include specifications for acceptable analyte identification, target analytes, and minimum and maximum percent recovery of the QA/QC compounds. Data are validated according to guidelines which set performance criteria for instrument calibration, analyte identification, and identification and recovery of QA/QC compounds. The *National Functional Guidelines for Data Review* (NFG), EPA validation, was designed for the assessment of data generated under the CLP analytical protocols.[5] The guidelines do not preclude the validation of field and other non-CLP data. Thus, many EPA Regions have also adapted the *National Functional Guidelines for Data Review* to validate non-CLP data. Data which do not meet the guidelines' performance criteria are qualified to indicate bias or QA/QC deficiencies. The data validation report usually explains why the data were qualified and indicates the bias direction when it can be determined. Validated data that are not qualified are considered unbiased and can be used at their reported numerical value for an HRS evaluation.

3 Superfund CLP Analytical Statements of Work are available at https://www.epa.gov/clp/superfund-clp-analytical-services. EPA SW-846 Compendium methods are available at https://www.epa.gov/hw-sw846/sw-846-compendium. CLP Guidance for Field Samplers is available at https://www.epa.gov/clp/clp-information-field-samplers.

4 See general descriptions of QC measures in Chapter 1 of the SW-846 Compendium.

5 The *National Functional Guidelines for Data Review* are available at https://www.epa.gov/clp/superfund-clp-national-functional-guidelines-nfgs-data-review.

QUALIFIER DEFINITIONS

Most EPA validation guidelines, such as the *National Functional Guidelines for Data Review*, use the data qualifiers presented in Exhibit 2. Other qualifiers besides these may be used; the validation report should always be checked for the exact list of qualifiers and their meanings.

It should be emphasized that not meeting one or some of the contract required QA/QC acceptance criteria is often an indication that the sample was difficult to analyze, not that there is low confidence in the analysis (i.e., the analysis is "under control" and can be adequate for HRS decision making). Often "J", "U", and "UJ" qualified data fall into this category.

There are instances when qualified data cannot be used since the uncertainty of the results is unknown. For example, some cases, such as certain violations of laboratory instrument calibration and tuning requirements, and gross violations of holding times, reflect the possibility that the results are of unknown quality (i.e., the analysis is "out of control"). Data that may be seriously affected by these deficiencies would be qualified with an "R" (not usable for HRS purposes).

"J" qualified data are generally considered biased, but provide definitive analyte identification. However, note that data qualified "J" solely due to detection at or above the detection limit but

EXHIBIT 2
EPA NFG DATA QUALIFIERS AND THEIR USABILITY FOR DOCUMENTING AN OBSERVED RELEASE

USABLE*	
"U"	The analyte was analyzed for, but was not detected above the level of the adjusted detection limit or quantitation limit, as appropriate.
"J"	The result is an estimated quantity. The associated numerical value is the approximate concentration of the analyte in the sample.
"J+"	The result is an estimated quantity, but the result may be biased high.
"J-"	The result is an estimated quantity, but the result may be biased low.
"UJ"	The analyte was analyzed for, but was not detected. The reported quantitation limit is approximate and may be inaccurate or imprecise.
NOT USABLE	
"NJ"	The analyte has been "tentatively identified", or considered "presumptively" present, and the associated numerical value is the estimated concentration in the sample.
"R"	The data are unusable. The sample results are rejected due to serious deficiencies in meeting QC criteria. The analyte may or may not be present in the sample.

* Usable under certain circumstances as explained in this fact sheet.

below the quantitation limit (not associated with other "J"-qualifying QC issues) are not considered to be biased. Other procedural qualifiers may be applied by the validator or appear in laboratory forms that do not imply any QC issue or bias (e.g., validator qualifiers like "C" or "X" identifying whether confirmatory analysis was performed, laboratory "D" qualifiers identifying a dilution was performed). Such qualifiers on their own do not require adjustment as described in this fact sheet. Furthermore, qualified data using alternative qualifiers and/or definitions different from those presented in the *National Functional Guidelines for Data Review* may be used and adjusted as needed based on requirements laid out in this fact sheet. However, using such qualified data should take into account the alternative qualifier definitions and how these correspond to qualifiers discussed in this fact sheet.

USING "U" QUALIFIED DATA

The "U" qualifier simply means that the reported concentration of the analyte was at or below the CRQL; there can be confidence that the true concentration is at or below the quantitation limit. Most often, this indicates that the analyte was not detected (i.e., its concentration is less than the MDL). Therefore, "U" qualified data can be used for establishing background levels. If the release sample concentration is above this level, as specified in the HRS, an observed release can be established.

USING "J" QUALIFIED DATA

As discussed previously, some "J" qualified data can be used in establishing an observed release if the uncertainty in the reported values is documented. Qualified data should always be carefully examined by the Regions to determine the reasons for qualification before use in an HRS evaluation. Whenever possible, qualified data should be used in conjunction with non-qualified data.

As described in Exhibit 2, "J" qualifiers indicate that bias has been detected in the sample analysis and although the analyte is definitively present, the reported concentration is an estimate. Depending on the reasons and the direction of bias, with the use of adjustment factors, "J" qualified data can represent data of known and documented quality sufficient for use in establishing an observed release under the HRS. "J" qualified data that are qualified solely due to detection at or above the detection limit but below the quantitation limit (not associated with other "J" qualifying QC issues) are not considered biased.

USING "UJ" QUALIFIED DATA

A combination of the "U" and "J" qualifiers indicates that the analyte was not detected, but the reported quantitation limit is approximate and may be inaccurate or imprecise. In nearly all instances, "UJ" qualifiers are applied to non-detected results (less than the detection limit [DL]) that are later found to be associated with a low bias QC issue (or an unknown biased QC issue, which includes the possibility of low bias). For such typical "UJ" qualified data, these data can be used as part of an HRS evaluation. Although some low bias may be associated with the original measurement, the non-detected result represents a measurement below the detection limit; there is typically a significant spread between the detection and quantitation limits (often a factor of 3 or more). Therefore, these "UJ" qualified data can be treated as non-detect for HRS purposes. Below are the procedures to be generally followed for use of "UJ" qualified data (in some cases, site-specific circumstances may dictate otherwise):

- Where the quantitation limit is available (the SQL, or CRQL for CLP data), treat the "UJ" qualified result as a normal non-detected result, and use the quantitation limit in determining observed release criteria.
- If the quantitation limit is not available, use the detection limit (e.g., the sample-specific MDL, or, for real-time field instruments, the detection limit of the instrument as used in the field). To compensate for the uncertainty of the measurement, multiply that detection limit value by three to generate a surrogate quantitation limit for use in determination of observed release criteria.

Under limited atypical conditions, "UJ" qualified data may not represent a not-detected result associated with low bias or unknown bias. Such atypical "UJ" qualified data can be used without adjustment to represent background concentrations for establishing an observed release under certain conditions. These conditions are: instances when there is confidence that the background concentration is not detectable above the CRQL, the background concentration is biased high, and the sample measurement establishing the observed release equals or exceeds the background sample CRQL.

DIRECTION OF BIAS IN "J" QUALIFIED DATA

It is important to understand the direction of bias associated with "J" qualified data before using the data to document an observed release. Qualified data may have high, low, or unknown bias. A low bias means that the reported concentration is likely an underestimate of the true concentration. For example, data may be biased low when sample holding times for volatile organic compounds (VOCs) are moderately exceeded or when recovery of QA/QC compounds is significantly less than the amount introduced into the sample. Low surrogate recovery would also indicate a low bias. A high bias means the reported concentration is likely an overestimate of the true concentration. For example, data may be biased high when recovery of QA/QC compounds is significantly higher than the amount in the sample. A bias is unknown when it is impossible to ascertain whether the concentration is an overestimate or an underestimate. For example, an unknown bias could result when surrogate recoveries exceed method recovery criteria and matrix spike/matrix spike duplicate compounds below method recovery criteria fail the relative percent difference (RPD) criteria in the same sample. Unknown bias generally includes the possibility of low bias and/or the possibility of high bias.

Despite the bias, certain qualified data may be used without application of adjustment factors for determining an observed release under certain circumstances. The following examples are of using "J" qualified data without adjustment factors:

- Low biased release samples are likely to be underestimates of true concentrations. If the reported concentration of a low biased release sample is three times above unbiased background levels, these release samples would still meet the HRS observed release criteria. The true concentrations would still be three times above the background level.
- High biased background samples are likely to be overestimates of true concentrations. If the reported concentration of unbiased release samples are three times above the reported background concentration, they would still meet the HRS observed release criteria because they would still be three times above the true background concentration.

The above examples show that both low bias "J" qualified release samples at their reported concentrations and high bias "J" qualified background samples may be used at their reported concentrations in these situations.

High biased release samples may not be used at their reported concentrations because they are an overestimate of true concentrations in this situation. The true difference in the background and release concentrations may be less than the HRS criteria for establishing an observed release. The reported concentration for low biased background concentrations may not be compared to release samples because it is most likely an underestimate of background level; the release sample concentration may not significantly exceed the true background concentration. However, high biased release data and low biased background data may be used with adjustment factors which compensate for the probable uncertainty in the analyses.

ADJUSTMENT FACTORS FOR BIASED "J" QUALIFIED DATA

Applying adjustment factors to "J" qualified data will enable EPA to be more confident that the increase in contaminant concentrations between the background and release samples is due to a release. The adjustment factors are applied as "safety factors" to compensate for analytical uncertainty, allowing biased data to be used for determining an observed release. The factors generally represent the ratio of the upper and lower bounds of anticipated performance for each analyte, based on the range of quality control percent recovery data used to generate them. (See the attachment section of this fact sheet for more detail.) Dividing a high biased result by an adjustment factor deflates it from the high end of the bounds towards the low end. Multiplying a low biased concentration by an adjustment factor inflates it to the high end of the bounds.

Adjustment factors do not correct the biased sample concentration to its true value because such "correction" is not possible. The quality control data used to derive adjustment factors do not differentiate and quantify individual sources of variation. Instead, the ratio of the upper and lower bounds of anticipated performance for each analyte used to develop adjustment factors represent a "worst-case" scenario. Adjustment factors either inflate background values to the high end of the range to generate an estimated maximum value or deflate release data to the low end to generate an estimated minimum value. Therefore, adjustment factors compensate, or adjust, for the apparent analytical variability when comparing a high biased value to a low biased value (see Exhibit 3). It should be noted that the adjustment factors reflect analytical variability; adjustment factors may still be applied to data that are assigned a "J" qualifier due to field sampling QC issues.

EXHIBIT 3
USE OF ADJUSTMENT FACTORS FOR "J" QUALIFIED DATA

TYPE OF SAMPLE	TYPE OF BIAS	ACTION REQUIRED
Background Sample	No Bias	None: Use concentration without factor
	Low Bias	Multiply concentration by factor
	High Bias	None: Use concentration without factor
	Unknown Bias	Multiply concentration by factor
Release Sample	No Bias	None: Use concentration without factor
	Low Bias	None: Use concentration without factor
	High Bias	Divide concentration by factor
	Unknown Bias	Divide concentration by factor

USING THE ADJUSTMENT FACTORS

This section of the fact sheet demonstrates how adjustment factors can be used with "J" qualified data for HRS scoring purposes, including documentation and detection limit issues.

Documentation Requirements for Using Qualified Data

In using "J" qualified data to determine an observed release, include a discussion of "J" qualifiers from the data validation report and cite it in the HRS documentation record as part of a reference. If adjustment factors are applied to "J" qualified data, reference and cite this fact sheet. These steps will ensure that the direction of bias is documented and will demonstrate how biases have been adjusted.

Application of Factors

Exhibit 3 shows how to apply the factors to "J" qualified data. Multiply low biased or unknown biased background sample results by the analyte-specific adjustment factor or the default factor 10 when an analyte-specific adjustment factor is not available. (This default of 10 may be applied for any analyte, method, or matrix that does not have a specific adjustment factor listed in the attachments to this fact sheet.) The resulting new background value effectively becomes a high biased value—an estimated maximum value that may be used to determine an observed release. Divide high biased release sample data by the analyte-specific adjustment factor or the default factor of 10 when an analyte-specific adjustment factor is not available. The resulting new release sample value effectively becomes a low biased value—an estimated minimum value that may be used to determine an observed release.

Note: High biased background data, low biased release data, and unbiased data may be used at their reported concentrations.

Note: Adjusted release and background values must still meet HRS criteria (e.g., release concentration must be at least three times above background level) to determine an observed release.

Examples Using Trichloroethene in Soil and Water

1. *Release water sample is unbiased, background water sample is unbiased, but all data are qualified with a "J" due to a contractual laboratory error, not an analytical error.*

   Background sample value: 12 micrograms per liter (µg/L) (J) *no bias*
   Release sample value: 40 µg/L (J) *no bias*

   The CRQL for trichloroethene is 10 micrograms per kilogram (µg/kg) for soil and 10 µg/L for water.

   In this example, the qualification of the data is not related to bias in the reported concentrations. Thus, using adjustment factors is not needed and an observed release is established if all other criteria are met.

2. *Release soil sample data are biased low, background soil sample data are biased high.*

   Background sample value: 12 µg/kg (J) *high bias*
   Release sample value: 40 µg/kg (J) *low bias*

In this example, the direction of bias indicates that the true release value may be higher and the true background value may be lower than reported values. The release sample concentration still exceeds background by more than three times, so an observed release is established, provided all other HRS criteria are met. Using adjustment factors is not needed.

3. *Release soil sample data are unbiased, background soil sample is biased low.*

   Background sample value: 12 µg/kg (J) *low bias*
   Release sample value: 30 µg/kg *no bias*

   In this example, the true background value is assumed to be greater than the reported value; however, an observed release may still be possible. To use the data to establish an observed release, multiply the background sample data value by the adjustment factor given for trichloroethene in soil (2.11). No adjustment factor is needed for the release sample.

   New background sample value:
   (12 µg/kg) x (2.11) = 25.32 µg/kg (J) *estimated maximum*

   The release sample concentration does not meet or exceed the new background level by three time, so an observed release is not established.

4. *Release water sample data are biased high, background water sample data are unbiased.*

   Background sample value: 15 µg/L *no bias*
   Release sample value: 70 µg/L (J) *high bias*

   In this example, the true release value may be lower than the reported value; however, an observed release may still be possible. To use the data to establish an observed release, divide the release sample by the adjustment factor for trichloroethene in water (1.66). No adjustment factor is needed for the background sample.

   New release sample value:
   (70 µg/L) ÷ (1.66) = 42.16 µg/L (J) *estimated minimum*

   The new release sample concentration does not meet or exceed the background level by three times, so an observed release is not established.

5. *Release soil sample data have unknown bias, background soil sample data have unknown bias.*

   The following example is the most conservative approach to using adjustment factors with qualified data.

   Background sample value: 20 µg/kg (J) *unknown bias*
   Release sample value: 325 µg/kg (J) *unknown bias*

In this example, the true release value may be lower than the reported value (because unknown bias includes the possibility of high bias), and the true background value may be higher than the reported value (because unknown bias includes the possibility of low bias); however, an observed release may still be possible. To use the data to establish an observed release, divide the release sample value and multiply the background sample value by the adjustment factor given for trichloroethene in soil (2.11).

New release sample value:
(325 µg/kg) ÷ (2.11) = 154.02 µg/kg (J) *estimated minimum*

New background sample value:
(20 µg/kg) x (2.11) = 42.2 µg/kg (J) *estimated maximum*

The new release sample is at least three times the new background concentration, so an observed release is established, provided all other HRS criteria are met.

6. *Release soil sample data are unbiased, background soil sample is "UJ" qualified due to low bias, SQL is available.*

   Background sample value: 12 µg/kg (UJ) *low bias, SQL = 12 µg/kg*
   Release sample value: *30 µg/kg no bias*

   In this example, the background value was originally reported as not detected, but "UJ" qualified due to low bias. The limit of 12 µg/kg associated with the reported UJ is the SQL. To use the data to establish an observed release, the "UJ" qualified background value is treated as a non-detect for HRS purposes, and the observed release criterion is set at 12 µg/kg. Because the release sample concentration equals or exceeds the background level SQL, an observed release is established.

7. *Release soil sample data are unbiased, background soil sample is "UJ" qualified due to low bias, MDL is available.*

   Background sample value: 3 µg/kg (UJ) *low bias, MDL = 3 µg/kg*
   Release sample value: 30 µg/kg *no bias*

   In this example, the background value was originally reported as not detected, but "UJ" qualified due to low bias. The limit of 3 µg/kg associated with the reported UJ is the MDL, and a quantitation limit is not available. To use the data to establish an observed release, the "UJ" qualified background value is treated as a non-detect for HRS purposes; because the quantitation limit is not available, the MDL is multiplied by three to generate a surrogate quantitation limit of 9 µg/kg to act as the observed release criterion. Because the release sample concentration equals or exceeds the background level surrogate quantitation limit, an observed release is established.

ISSUES WITH USING ADJUSTMENT FACTOR APPROACH

Some issues were raised regarding the application of adjustment factors to qualified data during the Agency's internal review process.

One issue is that "J" qualifiers are added to analytical results for many reasons that may or may not affect the accuracy and precision of the analytical result. The application of an adjustment factor to "J" qualified data in which bias is not affected could be considered overly conservative.

All qualified data should be carefully evaluated to determine if the data are biased. Based on the reasons for bias, the use of an adjustment factor should only be considered as a management tool that provides a quick screening of the data for site assessment, not a means for correcting the biased value to a true value. Application of adjustment factors are intended for use with biased qualified data and may not be applicable to data which are qualified but technically sound. As stated previously, qualified data should always be carefully reviewed on a case-by-case basis prior to use in an HRS evaluation.

Another issue is the validity of "10" as a default adjustment factor. A default adjustment factor of 10 was a policy decision based on the range of adjustment factors. The default was chosen in order to account for the maximum variability regardless of the direction of the bias. Therefore, the default value of 10 is generally considered to be a conservative adjustment factor. EPA reviewed the use of the default value of 10 and determined that this value was conservative.

Even if using adjustment factors is sometimes overly conservative, this approach is preferable to not using the data at all. EPA considers the use of adjustment factors appropriate as a management decision tool. However, discretion is needed when applying adjustment factors. The use of adjustment factors may not be appropriate in all cases.

USE OF OTHER ADJUSTMENT FACTORS

EPA Regions may substitute higher, but never lower, adjustment factor values for the ones listed in Attachment A of this fact sheet on a case-by-case basis when technically justified. For example, other adjustment factors may be applied to conform with site-specific Data Quality Objectives (DQOs) or with Regional Standard Operating Procedures (SOPs) (Data Quality Objectives Process for Superfund, Publication 9355.9-01).

SUMMARY

For site assessment purposes, EPA Regions should not automatically discard "J" qualified data. With careful assessment of the nature of the analytical biases or QC deficiencies in the data on a case-by-case basis, qualified data can represent an additional resource of data for establishing an observed release. However, site-specific data usability determinations may result in the data not being used.

Data qualified under the EPA's CLP or from other sources of validated data may be used to demonstrate an observed release if certain measures are taken to ensure that the bias of the data qualifier is adjusted using the factor approach specified in this fact sheet. (This fact sheet provides a management decision tool for making qualified data usable for documenting an observed release by chemical analysis, as well as for the purpose of identifying hazardous substances associated with a source where source samples are compared to background samples to demonstrate the relative increase in hazardous substance concentrations over background.) The analyte and matrix-specific adjustment factors provided in the attachment section of this fact sheet present these adjustment factors.

The scope of this fact sheet is limited to the situations described in Exhibit 1. The use of qualified analytical data without the adjustment factors presented in this fact sheet is limited. Higher adjustment factors may be substituted by EPA Regions on a case-by-case basis when technically justified by site-specific DQOs or SOPS.

REFERENCES

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ATTACHMENT A – Adjustment Factors for Soil and Water

Tables 1 through 4 present analyte and matrix-specific adjustment factors for soil (or sediment) and water samples to address the analytical uncertainty when determining an observed release by chemical analysis, or when identifying hazardous substances associated with a source in cases where contaminated source samples are compared to background samples; the adjustment factors are applied when using high biased or unknown biased release samples and/or low biased or unknown biased background samples. The factors were derived from percent recoveries of matrix spikes, surrogates, and laboratory control samples in the CLP Analytical Results Database (CARD) from January 1991 to March 1996. A total of 32,447 samples were reviewed for volatile organic analytes; 32,913 samples for semivolatile organic analytes; 59,508 samples for pesticides/PCB analytes; and 5,954 samples for inorganic analytes.

The range of CARD data for each analyte includes 97 percent of all percent recoveries in the database, removing the upper and lower 1.5 percent of the data distribution, which were expected to reflect extreme performance issues not expected to be representative of routine performance. The adjustment factors are ratios of percent recovery values at the 98.5 and 1.5 percentiles representing the bounds of anticipated performance for each analyte. The ratios generally show a consistent pattern.

Adjustment factors were determined for all analytes in the CLP Target Compound List (organic analytes) and Target Analyte List (inorganic analytes). For each organic analyte, an adjustment factor was derived from percent recoveries for surrogates and/or an adjustment factor was derived from percent recoveries for matrix spikes, as available. When both matrix spike and surrogate data were available for the same analyte, the larger adjustment factor (representing more extreme high and low percent recoveries) was used. Laboratory control samples were used to calculate the inorganic adjustment factors. Quarterly blind sample data were not used to determine adjustment factors because of the small data set available. A default adjustment factor of 10 was used for analytes when percent recovery data were unavailable.

TABLE 1 FACTORS FOR VOLATILE ORGANIC ANALYTES				
VOLATILE ORGANIC ANALYTES	Soil Matrix		Water Matrix	
	Number of CARD Samples Reviewed	Factor	Number of CARD Samples Reviewed	Factor
1,1,1-TRICHLOROETHANE	---	10.0	---	10.0
1,1,2,2-TETRACHLOROETHANE	---	10.0	---	10.0
1,1,2-TRICHLOROETHANE	---	10.0	---	10.0
1,1-DICHLOROETHANE	---	10.0	---	10.0
1,1-DICHLOROETHENE	7,031	2.71	5,015	2.35
1,2-DICHLOROETHANE-D4[6]	32,446	1.52	25,516	1.38
1,2-DICHLOROETHENE (TOTAL)	---	10.0	---	10.0
1,2-DICHLOROPROPANE	---	10.0	---	10.0
2-BUTANONE	---	10.0	---	10.0
2-HEXANONE	---	10.0	---	10.0
4-METHYL-2-PENTANONE	---	10.0	---	10.0
ACETONE	---	10.0	---	10.0
BENZENE	7,024	1.97	5,001	1.64
BROMODICHLOROMETHANE	---	10.0	--	10.0
BROMOFORM	---	10.0	---	10.0
BROMOFLUOROBENZENE	32,444	1.7	25,518	1.26
BROMOMETHANE	---	10.0	---	10.0
CARBON DISULFIDE	---	10.0	---	10.0
CARBON TETRACHLORIDE	---	10.0	---	10.0
CHLOROBENZENE	7,018	2.0	5,015	1.54
CHLOROETHANE	---	10.0	---	10.0
CHLOROFORM	---	10.0	---	10.0
CHLOROMETHANE	---	10.0	---	10.0
CIS-1,3-DICHLOROPROPENE	---	10.0	---	10.0
DIBROMOCHLOROMETHANE	---	10.0	---	10.0
ETHYLBENZENE	---	10.0	---	10.0
METHYLENE CHLORIDE	---	10.0	---	10.0
STYRENE	---	10.0	---	10.0
TETRACHLOROETHENE	---	10.0	---	10.0
TOLUENE-D8	32,447	1.63	25,526	1.21
TRANS-1,3-DICHLOROPROPENE	---	10.0	---	10.0
TRICHLOROETHENE	6,988	2.11	4,938	1.66
VINYL CHLORIDE	---	10.0	---	10.0
XYLENE (TOTAL)	---	10.0	---	10.0

6 Adjustment factors identified for deuterated versions of an analyte can also be used to adjust qualified data for non-deuterated forms of that analyte.

TABLE 2 FACTORS FOR SEMIVOLATILE ORGANIC ANALYTES				
SEMIVOLATILE ORGANIC ANALYTES	Soil Matrix		Water Matrix	
	Number of CARD Samples Reviewed	Factor	Number of CARD Samples Reviewed	Factor
1,2,4-TRICHLOROBENZENE	6,792	4.83	4,605	3.71
1,2-DICHLOROBENZENE-D4[7]	32,848	4.22	21,506	3.0
1,3-DICHLOROBENZENE	---	10.0	---	10.0
1,4-DICHLOROBENZENE	6,796	6.0	4,599	3.85
2,2'-OXYBIS(1-CHLOROPROPANE)	---	10.0	---	10.0
2,4,6-TRIBROMOPHENOL	32,605	9.38	21,509	3.57
2,4,5-TRICHLOROPHENOL	---	10.0	---	10.0
2,4,6-TRICHLOROPHENOL	---	10.0	---	10.0
2,4-DICHLOROPHENOL	---	10.0	---	10.0
2,4-DIMETHYLPHENOL	---	10.0	---	10.0
2,4-DINITROPHENOL	---	10.0	---	10.0
2,4-DINITROTOLUENE	6,798	4.88	4,623	3.52
2,6-DINITROTOLUENE	---	10.0	---	10.0
2-CHLORONAPHTHALENE	---	10.0	---	10.0
2-CHLOROPHENOL-D4	32,798	4.08	21,506	2.92
2-FLUOROBIPHENYL	32,913	3.38	21,532	2.84
2-FLUORPHENOL	32,781	5.05	21,511	3.34
2-METHYLNAPHTHALENE	---	10.0	---	10.0
2-METHYLPHENOL	---	10.0	---	10.0
2-NITROANILINE	---	10.0	---	10.0
2-NITROPHENOL	---	10.0	---	10.0
3,3'-DICHLOROBENZIDINE	---	10.0	---	10.0
3-NITROANILINE	---	10.0	---	10.0
4,6-DINITRO-2-METHYLPHENOL	---	10.0	---	10.0
4-BROMOPHENYL-PHENYLETHER	---	10.0	---	10.0
4-CHLORO-3-METHYLPHENOL	6,715	6.26	4,609	4.46
4-CHLOROANILINE	---	10.0	---	10.0
4-CHLOROPHENYL- PHENYLETHER	---	10.0	---	10.0
4-METHYLPHENOL	---	10.0	---	10.0
4-NITROANILINE	---	10.0	---	10.0
4-NITROPHENOL	6,627	9.33	4,586	5.96

7 Adjustment factors identified for deuterated versions of an analyte can also be used to adjust qualified data for non-deuterated forms of that analyte.

ACENAPHTHENE	6,773	4.68	4,600	3.63
ACENAPHTHYLENE	---	10.0	---	10.0
ANTHRACENE	---	10.0	---	10.0
BENZO(A)ANTHRACENE	---	10.0	---	10.0
BENZO(A)PYRENE	---	10.0	---	10.0
BENZO(B)FLUORANTHENE	---	10.0	---	10.0
BENZO(G,H,I)PERYLENE	---	10.0	---	10.0
BENZO(K)FLUORANTHENE	---	10.0	---	10.0
BIS(2-CHLOROETHOXY)METHANE	---	10.0	---	10.0
BIS(2-CHLOROETHYL)ETHER	---	10.0	---	10.0
BIS(2-ETHYLHEXYL)PHTHALATE	---	10.0	---	10.0
BUTYLBENZYLPHTHALATE	---	10.0	---	10.0
CARBAZOLE	---	10.0	---	10.0
CHRYSENE	---	10.0	---	10.0
DI-N-BUTYLPHTHALATE	---	10.0	---	10.0
DI-N-OCTYLPHTHALATE	---	10.0	---	10.0
DIBENZ(A,H)ANTHRACENE	---	10.0	---	10.0
DIBENZOFURAN	---	10.0	---	10.0
DIETHYLPHTHALATE	---	10.0	---	10.0
DIMETHYLPHTHALATE	—	10.0	---	10.0
FLUORANTHENE	---	10.0	---	10.0
FLUORENE	---	10.0	---	10.0
HEXACHLOROBENZENE	---	10.0	---	10.0
HEXACHLOROBUTADIENE	---	10.0	--	10.0
HEXACHLOROCYCLOPENTADIENE	---	10.0	---	10.0
HEXACHLOROETHANE	---	10.0	---	10.0
INDENO(1,2,3-CD)PYRENE	---	10.0	---	10.0
ISOPHORONE	---	10.0	---	10.0
N-NITROSO-DI-N-PROPYLAMINE	6,725	4.92	4,513	4.0
N-NITROSODIPHENYLAMINE	---	10.0	---	10.0
NAPHTHALENE	---	10.0	--	10.0
NITROBENZENE-D5	32,867	3.96	21,533	2.73
PENTACHLOROPHENOL	6,597	72.5	4,550	10.12
PHENANTHRENE	---	10.0	---	10.0
PHENOL-D5	32,855	3.85	21,489	3.53
PYRENE	6,543	11.86	4,612	5.67
TERPHENYL-D14	32,899	4.35	21,541	6.32

TABLE 3 FACTORS FOR PESTICIDES/PCB ANALTYES				
PESTICIDES/PCB ANALYTES	Soil Matrix		Water Matrix	
	Number of CARD Samples Reviewed	Factor	Number of CARD Samples Reviewed	Factor
4,4'-DDD	---	10.0	---	10.0
4,4'-DDE	---	10.0	---	10.0
4,4'-DDT	5,343	12.82	3,850	7.14
ALDRIN	5,526	14.26	3,829	6.63
ALPHA-BHC	---	10.0	---	10.0
ALPHA-CHLORDANE	---	10.0	---	10.0
AROCLOR-1016	---	10.0	---	10.0
AROCLOR-1221	---	10.0	---	10.0
AROCLOR-1232	---	10.0	---	10.0
AROCLOR-1242	---	10.0	---	10.0
AROCLOR-1248	---	10.0	---	10.0
AROCLOR-1254	---	10.0	---	10.0
AROCLOR-1260	---	10.0	---	10.0
BETA-BHC	---	10.0	---	10.0
DECACHLOROBIPHENYL	57,315	17.79	33,592	10.0
DELTA-BHC	---	10.0	---	10.0
DIELDRIN	5,539	11.93	3,861	4.87
ENDOSULFAN I	—	10.0	---	10.0
ENDOSULFAN II	—	10.0	---	10.0
ENDOSULFAN SULFATE	---	10.0	---	10.0
ENDRIN	5,521	14.13	3,850	5.33
ENDRIN ALDEHYDE	---	10.0	---	10.0
ENDRIN KETONE	---	10.0	---	10.0
GAMMA-BHC (LINDANE)	5,545	11.79	3,832	10.0
GAMMA-CHLORDANE	---	10.0	---	10.0
HEPTACHLOR	5,548	7.88	3,836	5.26
HEPTACHLOR EPOXIDE	---	10.0	---	10.0
METHOXYCHLOR	---	10.0	---	10.0
TETRACHLORO-M-XYLENE	59,508	8.5	33,787	5.29
TOXAPHENE	---	10.0	---	10.0

TABLE 4 FACTORS FOR INORGANIC ANALYTES				
INORGANIC ANALYTES	Soil Matrix		Water Matrix	
	Number of CARD Samples Reviewed	Factor	Number of CARD Samples Reviewed	Factor
ALUMINUM	5387	1.66	6208	1.30
ANTIMONY	5392	1.98	6170	1.27
ARSENIC	5675	1.74	6303	1.35
BARIUM	5360	3.99	6201	1.25
BERYLLIUM	5399	1.28	6208	1.25
CADMIUM	5385	1.41	6166	1.29
CALCIUM	5383	1.28	6201	1.24
CHROMIUM	5389	1.29	6210	1.30
COBALT	5392	1.25	6212	1.27
COPPER	5394	1.22	6205	1.25
CYANIDE	3281	1.55	225	1.36
IRON	5391	1.34	6216	1.27
LEAD	5982	1.44	6384	1.31
MAGNESIUM	5397	1.23	6210	1.24
MANGANESE	5395	1.24	6214	1.28
MERCURY	5954	1.83	256	1.50
NICKEL	5400	1.35	6210	1.29
POTASSIUM	3874	17.49	6175	1.24
SELENIUM	5620	2.38	6278	1.14
SILVER	5392	1.74	6215	1.42
SODIUM	5024	25.43	6195	1.26
THALLIUM	5621	1.86	6253	1.37
VANADIUM	5393	1.34	6212	1.25
ZINC	5404	1.50	6224	1.29