One Point Quality Control Precision and Bias
Graphics
For Criteria Pollutants

Companion Document

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1   Background

In order to provide decision makers with data of adequate quality, OAQPS is using the Data Quality Objective (DQO) process to determine our data quality needs for our ambient air criteria pollutants. There are some data quality indicators, such as precision, bias, and completeness that directly affect the attainment of the DQOs. These variables need to be in certain acceptable ranges (called measurement quality objectives) in order for us to make decisions (like comparison with the NAAQS) with specified levels of confidence. 40 CFR Part 58 Appendix A provides the minimum requirements for the collection and reporting of data to assess the data quality indicators of precision, bias, and completeness. On an annual basis, the Ambient Air Monitoring Group (AAMG) develop summary reports on these data quality indicators.

In 2006 OAQPS revised 40 CFR Part 58 Appendix A in order to base the precision and bias measurement quality objectives on confidence intervals at the site level of data aggregation. Since the criteria pollutant data are used for very important decisions (comparison to the NAAQS) it is felt that providing precision and bias estimates at upper confidence limits provides a higher probability of making appropriate decisions. This statistic provides a conservative approach to measuring precision and bias. A document describing these statistics is available on AMTIC. (http://www.epa.gov/ttn/amtic/parslist.html)

Estimates of both bias and precision for the four automated gaseous methods (CO, NO_2, O_3, and SO_2) are derived from the bi-weekly one-point QC checks. Since every site should perform the QC checks at an acceptable frequency, there is enough information to assess and control data quality at the site level.

In 2005, OAQPS developed a new report in AQS (AMP255 – P/A Quality Indicator Summary Report) that summarized precision, bias, and completeness of the required QC data for each criteria pollutant. The data tables may be generated at any time within the AQS application using the standard report. Earlier reports also generated this data graphically which monitoring organizations found very useful. Since AQS presently does not have this capability, AAMG is providing these graphs annually as an addendum to the summary tables. The AMP255 was later updated and replaced by the AMP256 report

This document defines the elements displayed in the corresponding box and whisker graphics as well as base assumptions of the data contained within the AMP256 report.
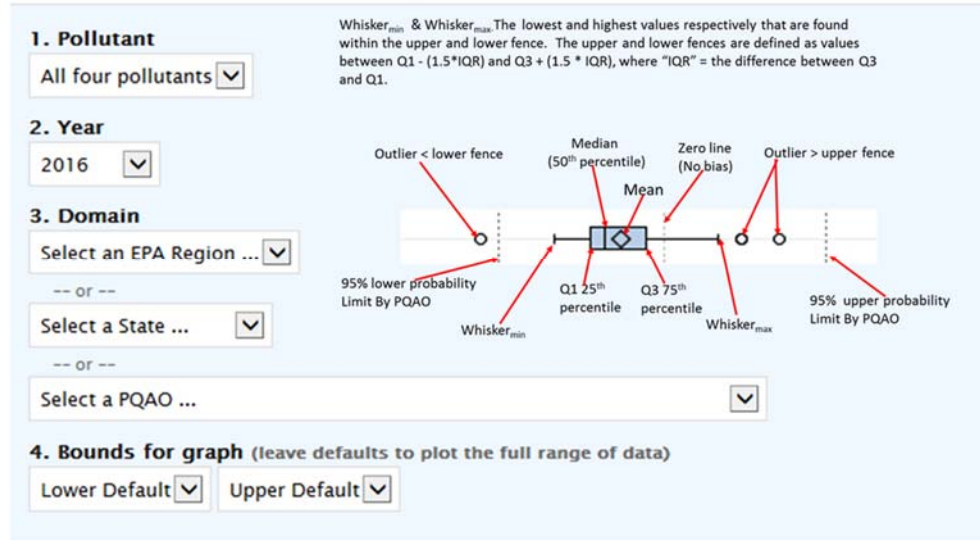
1.1   Generating the Report

Go to the following website https://www.epa.gov/air-data/single-point-precision-and-bias-report.   It will bring you to the Single Point Precision and Bias Report (***Figure 1)*. From this page you can select individual gaseous criteria pollutants or all four. You can then select a year and one of three domains: 1) an EPA Region, 2) a State or, 3) a PQAO. You can also select the "bounds for graph". Its use is discussed in section 2.2.19. Once you've made your selection, hit the "Plot Data" button.

Fig 1. Selection Criteria for Box and Whisker Plots

2 Report Description

2.1 Components of the Graphs

2.1.1 Overview

Each graph presented in the *s* is comprised of four parts. Each of these parts are discussed in the following sections. The four parts of each graph are as follows:

- Data Grouping
- Supplemental Statistics
- Box and Whisker Plots
- 95% CFR Confidence Limits

Figure 2 illustrates how these different components appear within each graph.
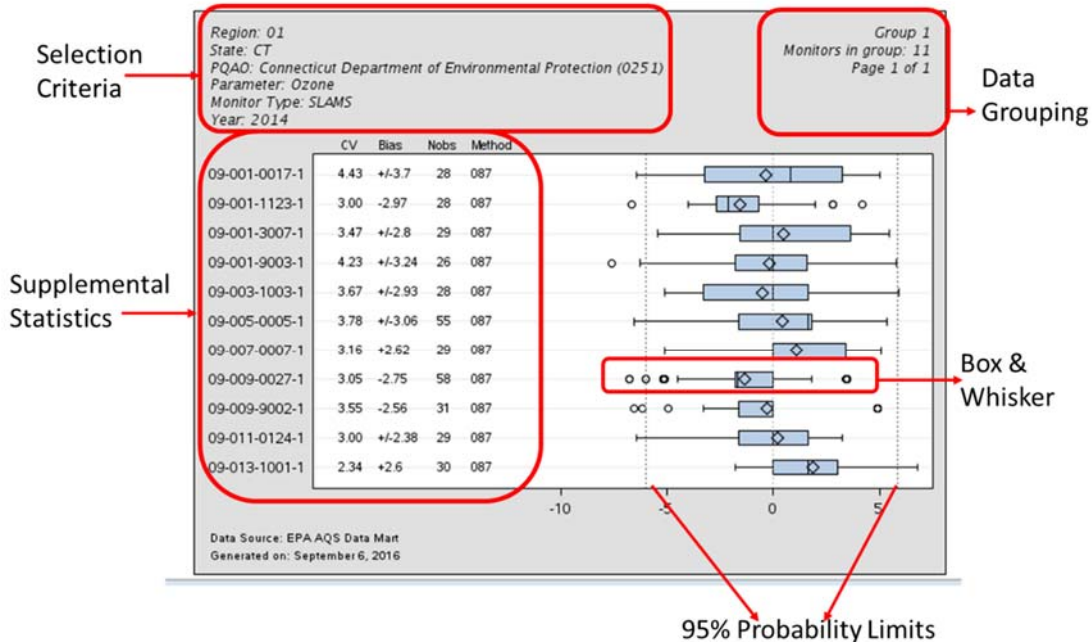
Figure 2. Components of Box and Whisker Plots

A given page will display up to 12 box plots.

2.1.2 Data Grouping (upper right hand corner)

Each page of the report displays the results for a particular data grouping. A "data grouping" is defined by unique combinations of Domain (Region or State or PQAO) and Monitor Type Classification. However, once the report is generated, the data is output by PQAO and monitor type classification. For example, if one selected a state that had four PQAOs all with SLAMs monitor type classifications and two of those PQAOs also had an "SPM" monitor type classification, the evaluation would display a total of 6 groupings. Each report identifies the number of monitors in that group as well as the number of pages in the group. If a PQAO has more than 12 monitors measuring the same pollutant for the same monitor type classification, the graphs will appear on multiple pages.

2.1.3 Supplemental Statistics

In addition to the statistics represented in the box and whisker, the following information and statistics are displayed for each monitor within each data grouping:

- AQS ID – The plots are sorted by the AQS ID in ascending order.
- CV Upper Bound
- Bias Upper Bound
- # Obs - Number of Samples contained within the set
- Method Designation

The information displayed in this area of the plots would also be found in the AMP256 Report.

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2.1.4 Box and Whisker Plots

A "Box and Whisker Plot" is created for each monitor within a reporting organization measuring a gaseous criteria pollutant (carbon monoxide, nitrogen dioxide, ozone, and sulfur dioxide). A single box plot is based on the percent relative error statistics from the one-point precision checks for a single monitoring site measuring a pollutant conducted within the effective time period in 2013. Multiple box plots are displayed within a data grouping. A box plot displays the following statistics:

- Q3 (75th Percentile)
- Q2 (50th Percentile) - Median
- Q1 (25th Percentile)
- Arithmetic Mean
- Whiskermin & Whiskermax The lowest and highest values respectively that are found within the upper and lower fence. The upper and lower fences are defined as values between Q1 - (1.5*IQR) and Q3 + (1.5 * IQR), where "IQR" = the difference between Q3 and Q1.
- Outliers: All values that fall outside the upper and lower fences.

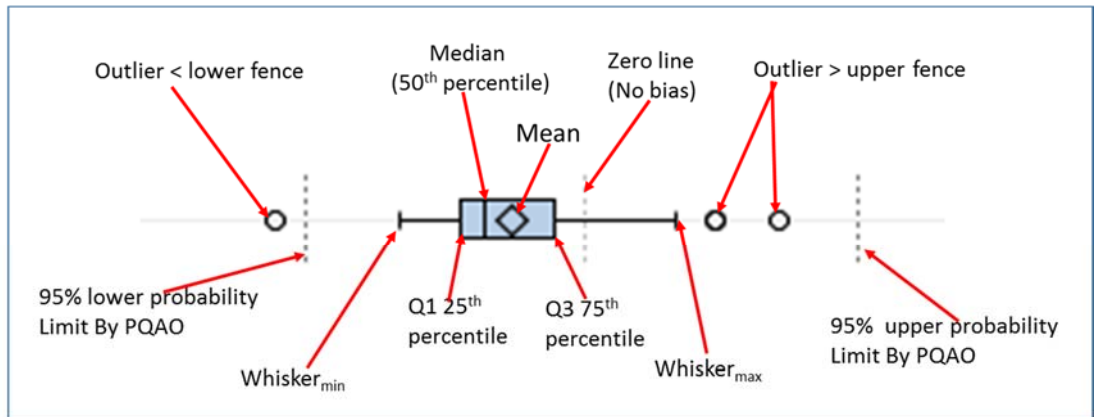The statistics are represented according to **Figure 3**.

Figure 3 - Components of a Schematic Box and Whisker Plot

2.1.5 95% CFR Limits

The following statistics are calculated for all Pollutant - monitor type category - monitors within the PQAO:

- 95% CFR Upper Probability Limit
- 95% CFR Lower Probability Limit

The 95% Probability Limits are displayed as vertical dashed line within the box and whisker plots.

2.2 Definitions for Each of the Displayed Items

The data grouping is a unique combination of a Region, State, Agency, Pollutant, and Monitor Type Classification. The data grouping for each box plot appears at the top of each page.

2.2.1 Region
The USEPA Region code associated with a given monitoring site.

2.2.2 State
A 2-character postal abbreviation is used to identify a state in which the monitoring site is located.

2.2.3 Primary Quality Assurance Organization (PQAO)
This is the description for the PQAO along with its corresponding PQAO code in parenthesis. The PQAO is the organization responsible for the quality assurance information submitted to AQS.

2.2.4 Parameter
This is the gaseous pollutant under consideration.

2.2.5 Monitor Type Classifications
Each monitor type will be grouped separately. Monitor types include EPA, INDUSTRIAL, NON-EPA FEDERAL, OTHER, SLAMS, SPM, TRIBAL.

2.2.6 Year
The calendar year the data was collected

2.2.7 AQS Site ID
The AQS Site ID (State code, County code, and AQS Site ID) combined with the Pollutant Occurrence Code (POC) used to uniquely define a monitor within the AQS database. The AQS ID appears in the top block of statistics as well as along the x-axis of the graph.

2.2.8 Pollutant Occurrence Code (POC)
The identifier used to distinguish between multiple monitors at the same site that are measuring the same parameter.

2.2.9 CV Upper Bound

Equations from this section come from *CFR Pt. 58, App. A, Section 4, "Calculations for Data Quality Assessment"*. For each single point check, calculate the percent difference, d_i, as follows:

Equation 1

$$d_i = \frac{meas - audit}{audit} \cdot 100$$

where *meas* is the concentration indicated by the monitoring organization's instrument and *audit* is the audit concentration of the standard used in the QC check being measured.
The precision estimate is used to assess the one-point QC checks for gaseous pollutants described in section 3.2.1 of CFR Part 58, Appendix A. The precision estimator is the coefficient of variation upper bound and is calculated using Equation 2 as follows:

Equation 2

$$CV = \sqrt{\frac{n \cdot \sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} d_i\right)^2}{n(n-1)}} \cdot \sqrt{\frac{n-1}{\chi_{0.1,n-1}^2}}$$

where $\chi^2_{0.1,n-1}$ is the 10th percentile of a chi-squared distribution with *n-1* degrees of freedom.

2.2.10   Bias

The bias estimate is calculated using the one point QC checks for SO_2, NO_2, O_3, or CO described in CFR, section 3.2.1. The bias estimator is an upper bound on the mean absolute value of the percent differences (see equation 1) as described in Equation 3 as follows:

Equation 3

$$|bias| = AB + t_{0.95,n-1} \cdot \frac{AS}{\sqrt{n}}$$

where *n* is the number of single point checks being aggregated; $t_{0.95,n-1}$ is the 95th quantile of a t-distribution with n-1 degrees of freedom; the quantity *AB* is the mean of the absolute values of the d_i's (calculated by Equation 1) and is expressed as Equation 4 as follows:

Equation 4

$$AB = \frac{1}{n} \cdot \sum_{i=1}^{n} |a$$

and the quantity *AS* is the standard deviation of the absolute value of the d_i's and is calculated using Equation 5 as follows:

Equation 5

$$AS = \sqrt{\frac{n \cdot \sum_{i=1}^{n} |d_i|^2 - \left(\sum_{i=1}^{n} |d_i|\right)^2}{n(n-1)}}$$

2.2.10.1 Sign Association for Absolute Bias

Since the bias statistic as calculated in Equation 3 of this document uses absolute values, it does not have a tendency (negative or positive bias) associated with it. A sign will be designated by rank ordering the percent differences (d_i's) of the QC check samples from a given site for a particular assessment interval and identifying the 25th and 75th percentiles of the percent differences. The absolute bias upper bound should be flagged as positive if both percentiles are positive and negative if both percentiles are negative. The absolute bias upper bound would not be flagged if the 25th and 75th percentiles are of different signs (i.e. straddling zero).

2.2.11   # Obs

The number of samples is the number of valued pairs of 1-point QC check data used within the calculation. The number should be represented on the graphic with an "n".

2.2.12   Method

The three digit method designation of the monitor for the particular Site ID and POC and is related to the Federal Reference Method (FEM) or Federal Equivalent Method (FEM). These codes (last three digits) with additional descriptions can be found on AMTIC[1].

2.2.13   Quartiles (Q1, Q2, Q3)

The quartiles are the 25th, 50th, and 75th percentiles respectively. Each of these values is represented within the lines of the box on the box plot. The Q1 value is the lowest line on the box. The Q2 value is the line within the box and the Q3 value is the top line of the box.

2.2.14   Mean

The mean is the average value of the percent differences within the dataset.

$$Mean = \frac{1}{n} \times \sum_{i=1}^{n} \left(100 \times \frac{(ind_i - act_i)}{act_i}\right)$$

where "*d*" is the percent difference for a given observations, and "*n*" is the total number of observations within the dataset. The value of the mean is represented by a plus sign (+) on the box plot.

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[1] List of Designated Reference and Equivalent Methods at http://www.epa.gov/ttn/amtic/criteria.html

2.2.15 Whisker$_{min}$ and Whisker$_{max}$

The Inter-Quartile Range (IQR) is defined as the difference between Q3 and Q1. The Whisker$_{min}$ is defined as the smallest value that is greater than or equal to Q1 – (1.5*IQR). The Whisker$_{max}$ is defined as the largest value that is less than or equal to Q3 + (1.5*IQR). The Whisker$_{min}$ and Whisker$_{max}$ values define the lengths of the "whiskers" that extend above and below the box. The ends of the whiskers are terminated with a horizontal line.

2.2.16 Outliers

Any value that is less than Q1 – (1.5*IQR) or any value that is greater than Q3 + (1.5*IQR) is defined as an outlier. All outliers are plotted on the graph. Outliers are represented by an "O".

2.2.17 95 % CFR Upper/Lower Probability Limits

The CFR Upper / Lower Probability Limits give the 95% probability limits of percent difference values for the time period for a given data grouping. The probability limits are calculated as follows:

*CFR Upper Probability Limit = D + (1.96 * s)*
*CFR Lower Probability Limit = D - (1.96 * s)*

where *D* and *s* are the respective mean and standard deviation of percent differences for the data grouping.

2.2.18 Percent Difference

The statistics are based on the percent difference values calculated from single point QC checks. Percent difference expresses the difference between the pollutant concentration indicated by monitoring equipment and the known concentration of the sample used in the check. The percent difference is calculated as:

$$d = 100 * \frac{(indicated - actual)}{actual}$$

where d is percent difference, indicated is the value obtained from the monitor, and actual is the known concentration level.

2.2.19   Use of "Bounds for Graph" Selection

Since outliers will be displayed, they dictate how the box and whisker plots are generated. Single large outliers can condense the plot size making the plots virtually unreadable. However, they can help to identify possible errors in data entry or data that should have been invalidated. An example of this follows. *Figure 4* represents a plot with the bound of graph at default (all outliers shown). The -100% difference for one QC check dictate the size of the box and whisker for the group. It is suggested that the plots initially be reviewed in default to identify outliers for potential correction action. *Figure 5* is the same set of data with the bounds set to +10% and -10%.
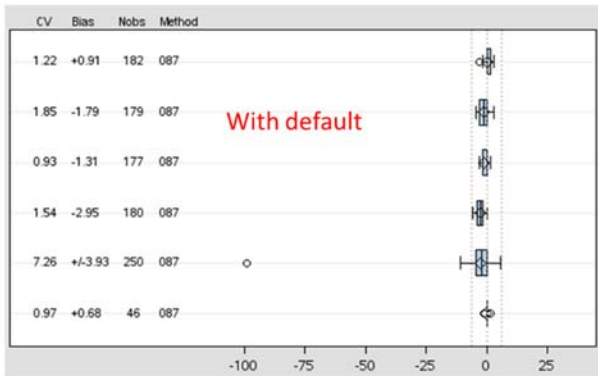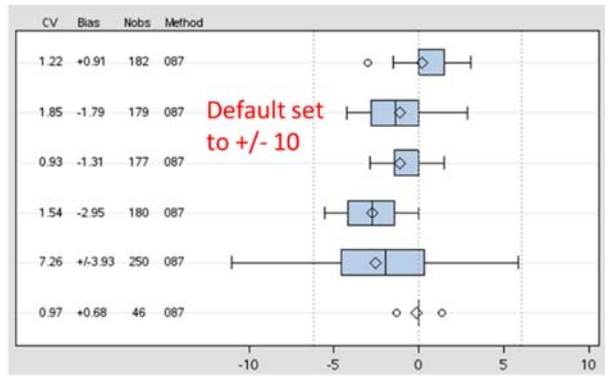

Figure 4. Plots with default

Figure 5 with defaults set to ± 10%