Advanced Retrievals

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Outline

- Course objectives
- Design Value Report
- Raw Data Qualifier Report
- Questions and answers

Course Objectives

1. To explain the contents of the two most complex AQS reports:
   - Design Value Report (AMP480)
   - Data Quality Indicator Report (AMP255)
2. To provide opportunity for feedback and suggested enhancements to the reports discussed.

Design Value Report

- Background
- Common features
- Pollutant specific features
- Questions and answers

What is a Design Value

- Design Values are the metrics (i.e. statistics) that are compared to the National Ambient Air Quality Standards (NAAQS) to determine compliance with the Federal regulations for air quality (40 CFR Part 50). (see http://www.epa.gov/air/criteria.html)
- The "form" of each Design Value, e.g. averaging time, is specific to each criteria pollutant. For pollutants with more than one NAAQS, there is a distinct design value for each NAAQS.
- Data handling issues, such as number of digits after decimal and rounding or truncating, are specified in Part 50.

Exceptional Events

- The Design Value report provides three options for displaying values flagged as affected by exceptional events:
  - Exclude flagged values that are concurred by the EPA
  - Exclude all flagged values
  - Do not exclude any flagged values

Report Purpose

- The purpose of this report is to provide the capability to calculate the 3-year Design Values for a selected set of monitors and years.
- Pollutants where 1-year statistics are used for NAAQS Determinations are not included on the report. (they are provided by the Quick Look Report)

Pollutants With 3-Year Standards

- Ozone
- PM 10
- PM 2.5
- NO2
- SO2
- Lead

Common Features

- Each pollutant has its own specific report and workfile format
- Each pollutant has its own DV folder in Discoverer
- The report shows a snapshot of the state of the AQS database at the time it was run (i.e. it may display preliminary or incomplete data)
- Intermediate calculations are shown to allow the user to determine how the design value and its validity are determined.

Ozone: DV Statistics

- There are two NAAQS standards in effect for 8-hour Ozone – the 1997 standard and the 2008 standard.
- Design Values are calculated for Monitors (rather than Sites)
- The 3-year Design Value is the mean of the annual 4th highest daily maximum 8-hour average
  - For both the 1997 and 2008 standards, the design value is computed to 3 digits after the decimal with additional digits truncated.
  - For the 1997 standard the 3rd digit is then rounded (values < 5 rounded down and values >= 5 rounded up)

Ozone: Validity

- The 3-year design value is marked as valid if three consecutive years of data are available and the following criteria are met:
  - The 3-year completeness is greater than or equal to 90% and at least one of the following is true for each of the 3 years:
    - The annual completeness is at least 75%
    - The annual 4th maximum is greater than the level of the standard

    OR
  - The 3-year average of the annual 4th maxima is greater than the level of the standard.

PM 2.5: DV Statistics

- There are two NAAQS Standards for PM 2.5 – An annual standard and a 24-hour standard
  - The annual standard is the 3-year average of the weighted annual arithmetic means of each of the years (rounded to 1 digit after decimal)
  - The 24-hour standard is the 3-year average of the 98th percentiles of each of the years (rounded to zero digits after decimal)

PM 2.5: Site Statistics

- Design values are calculated from daily values at the site-level (as distinct from the monitor level)
  - If a measurement is taken at the primary monitor at a site, it is the site value for the day.
  - If no value is taken at the primary monitor, then the site value is the average of the values at the collocated monitors at the site.
- AQS does not compute spatially averaged design values.

PM 2.5: 24-Hour DV Validity

- The 24-hour design value is marked as complete if there are 3 consecutive years of data and any of the following are met:
  - The 3-year design value is greater than the level of the standard
  - All quarters are at least 75% complete
  - For any year with quarters that are less than 75% complete, the annual 98th percentile value is greater than the level of the standard.

PM 2.5: Annual DV Validity

- The annual design value is marked as complete if all three years are present and any of the following criteria are met:
  - Each calendar quarter is at least 75% complete
  - All quarters have at least 11 values and the corresponding annual mean or 3-year DV is greater than the level of the standard.
  - For any quarter with less than 11 values, substituting the 3-year minimum for the same calendar quarter for the missing values would result in a 3-year DV greater than the level of the standard.

PM 2.5: Substituted Means

- AQS computes a set of "substituted means" that are provided in the workfile and Discoverer.
  - Quarterly substituted mean: For quarters with less than 11 values: Substitute for the missing values the minimum daily average for that quarter from the 3-year period to get a total of 11 values.
  - Annual substituted mean: For years with incomplete quarters, average the substituted quarterly means where present and quarterly means where not.
  - 3-Year substituted mean: For 3-year periods with substituted annual means, average the substituted annual means where present and annual means where not.

PM 10: DV Statistics

- From 40 CFR Part 50.6: The standards are attained when the expected number of days per calendar year with a 24-hour average concentration above 150 µg/m3 is equal to or less than one.
- The design value statistic is the 3-year average of the annual expected number of exceedances.

PM 10: Definitions

- Expected Exceedances: If PM10 sampling is scheduled less frequently than every day, or if some scheduled samples are missed, a PM10 value will not be available for each day of the year. To account for the effect of incomplete data, an adjustment is made to the data collected at each monitoring location to estimate the number of exceedances in a calendar year. It is assumed that the fraction of missing values that would have exceeded the standard level is identical to the fraction of measured values above this level.

PM 10: Calculations

- Estimated exceedances are calculated quarterly, and then summed for the year.
- Estimated exceedance = Actual number of exceedances X (number of days in quarter / number of sampled days in quarter). Example if there is one actual exceedance in a quarter with complete one-in-six sampling, then the estimated exceedance count would be 6.
- Rounding: Quarterly estimates are rounded to 2 digits and annual estimates are rounded to 1.

PM 10: Exceptions

- If the exceedance is the first (ever) for the monitor, it will not be adjusted if every day sampling is initiated and maintained for 4 calendar quarters.

PM 10: Validity

- The 3-year design value is marked as valid if three consecutive years of data are available and if either of the following criteria are met:
  - Observation Percent >= 75% for each quarter for all 3 years
  - 3-Year Estimated Exceedances > 1

NO2: DV Statistics

- There are two NAAQS Standards for NO2 – An annual standard and a 1-hour standard
  - The annual standard design value is the single-year annual arithmetic mean of all hourly values for the year (not shown on report).
  - The 1-hour standard design value is the 3-year average of the annual 98th percentiles of the daily maxima.
    - The 1-hour standard will be calculated at the site-level (as distinct from the monitor-level). AQS requires a primary monitor to be designated at each NO2 site, and only data from the primary monitor will be utilized for design value calculations.

NO2: Calculations

- Two distinct annual 98th percentile values are calculated for each year, as shown below, and the highest is used as the annual value:
  - The 98th percentile is taken from the set of daily maxima of valid days (days with 18 or more samples) .
  - The 98th percentile is taken from the set of daily maxima for all days with at least 1 sample.

NO2: Validity

- The 1-hour design value is marked as valid if any of the following criteria are met:
  - All quarters in the 3-year period are at least 75% complete.
  - At least 75 percent of the days in each quarter have at least one reported hourly value, and the design value is above the level of the standard.
  - The design value is less than the level of the standard and passes the “high value test” below.
  - The design value is above the level of the standard and passes the “low value test” below.

NO2: High Value Test

- For the quarter that is less than 75% complete:
  - There must be at least 200 valid days across all 3 years for that quarter.
  - Each corresponding quarter must be at least 50% complete.
  - The number of missing days below 75% shall have as their substitution value the largest daily maximum across **all** days in the corresponding calendar quarter across all 3 years. If the 3-year average of the annual 98th percentiles of this set is below the level of the standard, then the test is passed.

NO2: Low Value Test

- For the quarter that is less than 75% complete:
  - There must be at least 200 valid days across all 3 years for that quarter.
  - The number of missing days below 75% shall have as their substitution value the **minimum** daily maximum across **valid** days in the corresponding calendar quarter across all 3 years. If the 3-year average of the annual 98th percentiles of this set is above the level of the standard, then the test is passed.

SO2: DV Statistics

- The 1-hour standard design value for SO2 is the 3-year average of the annual 99th percentile values of the daily maxima.
- Design values are calculated at the site-level (as distinct from the monitor-level). Where there are multiple monitors at a site, for each year AQS uses the monitor with the highest average quarterly completeness. In the event that two monitors have the same average quarterly completeness, AQS uses the one with the smallest POC.

SO2: Calculations

- Two distinct annual 99th percentile values are calculated for each year, as shown below, and the highest is used as the annual value:
  - The 99th percentile is taken from the set of daily maxima of **valid** days (days with 18 or more samples).
  - The 99th percentile is taken from the set of daily maxima for **all** days with at least 1 sample.

SO2: Validity

- The 1-hour design value is marked as valid if any of the following criteria are met:
  - All quarters in the 3-year period are at least 75% complete
  - At least 75 percent of the days in each quarter have at least one reported hourly value, and the design value is above the level of the standard.
  - The design value is less than the level of the standard and passes the “high value test” below.
  - The design value is above the level of the standard and passes the “low value test” below

SO2: High Value Test

- For the quarter that is less than 75% complete:
  - There must be at least 200 valid days across all 3 years for that quarter
  - Each corresponding quarter must be at least 50% complete
  - The number of missing days below 75% shall have as their substitution value the largest daily maximum across **all** days in the corresponding calendar quarter across all 3 years. If the 3-year average of the annual 98th percentiles of this set is below the level of the standard, then the test is passed.

SO2: Low Value Test

- For the quarter that is less than 75% complete:
  - There must be at least 200 valid days across all 3 years for that quarter
  - The number of missing days below 75% shall have as their substitution value the **minimum** daily maximum across **valid** days in the corresponding calendar quarter across all 3 years. If the 3-year average of the annual 98th percentiles of this set is above the level of the standard, then the test is passed.

Lead: DV Statistics

- The design value for lead is the maximum 3-month average of the monthly mean concentrations for the 3-year period.
  - The month associated with each 3-month rolling average is the 3rd month of the period (e.g. the month for the average of January, February, and March is March).
  - Each 3-month average is rounded to 2 digits after the decimal.

Lead: Site Statistics

- Lead design values are calculated from daily values at the site-level (as distinct from the monitor level)
  - If a measurement is taken at the primary monitor at a site, it is the site value for the day.
  - If no value is taken at the primary monitor, then the site value is the average of the values at the collocated monitors at the site.

Lead: AQS DV Parameters

- Lead Design Values can be calculated from a combination of data from Pb-TSP/LC (14129), Pb-PM10/LC (85149), and Pb-TSP/STP (12128)
  - If valid 3-month Pb-PM10 averageshows a violation and is either greater than the 3-month Pb-TSP mean or there is no corresponding valid 3-month Pb-TSP mean present, then that 3-month Pb-PM10 mean will be the site-level mean for that 3-month period.
  - Prior to 2009, if only Pb-TSP/STP (12128) is present, it is utilized to compute the site-level 3-month means (with no adjustments for STP vs LC)

Lead: DV Validity

- The Lead design value is marked as valid if any of the following criteria are met:
  - It is above the level of the standard.
  - There are 36 valid 3-month averages for the 3-year period. A 3-month average is considered valid if it meets any of the following criteria:
    - If each month in the period is 75% complete.
    - It passes either the above NAAQS or below NAAQS tests defined below

Lead: Above NAAQS Test

- The 3-month average must be above the level of the standard.
- Data substitution will be done in each month of the 3-month period that is less than 75% complete.
- The substitution value is the lowest reported daily value for the corresponding month in the 3-year period.
- The test passes if by substituting enough values in the month for it to be 75% complete, the 3-month average is above the level of the standard.

Lead: Below NAAQS Test

- The 3-month average must be below the level of the standard.
- Data substitution will be done in each month of the 3-month period that is less than 75% complete but at least 50%.
- The substitution value is the highest reported daily value for the corresponding month in the 3-year period.
- The test passes if by substituting enough values in the month for it to be 100% complete, the 3-month average is below the level of the standard.

Data Quality Indicator Report (AMP255)

- Background – 40 CFR Part 58 Appendix A
- One Point Quality Control Check for Gases
- Annual Performance Evaluation for Gases
- Flow Rate Verification for PM and Lead
- Semi-Annual Flow Rate Audit for PM and Lead
- Collocated Audits for PM and Lead
- Performance Evaluation Program for PM and Lead
- Lead Analysis Audits

Background (1)

- 40 CFR Part 58 Appendix A contains the regulatory requirements for monitoring QA
  - The AQS Data Quality Indicator Report, AMP255, implements the assessments defined in Appendix A.
  - The report presents completeness, precision, and bias statistics for these assessments.
  - This AQS faciltiy provides both a print-formatted report and workfiles for importing into Excel (note: Currently, there is a problem with the Excel files).
  - Summarizes data reported on QA/QC transactions (RP and RA transactions) and computed for collocated monitors (from RD transactions)

Background (2)

- The report is used as part of the certification process.
- The report separately presents data for "Regulatory" monitors vs Non-Regulatory monitors. Non-Regulatory monitors are those with a monitor type set to "NON REGULATORY"
  - Non-regulatory monitors are labeled with "App A?: No"
  - All others are labeled with "App A?: Yes"

Calculations: Relative Percent Difference

- Basis for all statistical calculations
- For Gases:

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

- For Collocated Samples (including PEP):

$$d_i = \frac{X_i - Y_i}{(X_i + Y_i)/2} \bullet 100$$

  - Where X_i is the primary sample and Y_i is the collocated sample

One Point QC Check (1)

- A one-point quality control (QC) check must be performed at least once every 2 weeks on each automated analyzer used to measure SO_2, NO_2, O_3 and CO.
- Report is organized by pollutant and regulatory/non-regulatory
- Detail data is presented by Monitor and summarized first by year then by PQAO.
- Monitor detail Begin and End dates are the intersection of report date range, Sample Period, and PQAO assignment
- Number required reflects CFR specifying assessments every 2 weeks for date range
- Number of Observation is number of Gaseous RP transactions loaded in date range

One Point QC Check (2)

- Coefficient of Variation (precision estimate)

$$CV = \sqrt{\frac{n \bullet \sum_{i=1}^{n} d_i^2 - (\sum_{i=1}^{n} d_i)^2}{n(n-1)}} \bullet \sqrt{\frac{n-1}{\chi^2_{0.1,n-1}}}$$

Chi-Squared Distribution

- Bias

$$Bias\_Estimate = \frac{1}{n} \bullet \sum_{i=1}^{n} |d_i| + t_{0.95,n-1} \bullet \frac{AS}{\sqrt{n}}$$

Standard Error

Student-t Distribution

  - Where

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

One Point QC Check (3)

- Sign of Bias
  - If the 25th percentile of the relative percent difference and 75 percentile are both negative, then the sign of the bias is negative.
  - If the 25th percentile and 75th percentile are both positive, then the sign of the bias is positive.
  - If the 25th percentile is negative and the 75th percentile is positive, then the sign of the bias is undetermined (+/-)

Annual Perfomance Evaluation (1)

- Each calendar quarter (during which analyzers are operated), evaluate at least 25 percent of the SLAMS analyzers that monitor for SO_2, NO_2, O_3, or CO such that each analyzer is evaluated at least once per year.
- Report is organized by pollutant
- Detail data is presented by Monitor and summarized first by year then by PQAO.
- Monitor detail Begin and End dates are the intersection of report date range, Sample Period, and PQAO assignment
- Average Percent Difference is displayed by Audit Level (levels 1 – 10)

Annual Perfomance Evaluation (2)

- "Obs / Q" is the number of RA transactions submitted for each quarter
- "Criteria Met?" Is determined by the CFR requirement for one audit per site with 3 levels each year

Annual Perfomance Evaluation (3)

- Confidence limits are on the mean relative percent difference of the **1-point QC Checks**:
  - Upper 95% Confidence Limit = Mean + 1.96 * Standard_Deviation
  - Lower 95% Confidence Limit = Mean – 1.96 * Standard_Deviation
  - These are displayed only for summary rows (year and PQAO)
- The report also computes the percent of the **Annual PE** percent differences between the confidence limits on the **1-point QC Checks**

Flow Rate Verifications (1)

- A one-point flow rate verification check must be performed at least once every month on each automated analyzer used to measure PM_{10}, $PM_{10-2.5}$and $PM_{2.5}$. (TSP is quarterly)
- Report is organized by pollutant
- Detail data is presented by Monitor and summarized first by year then by PQAO.
- Monitor detail Begin and End dates are the intersection of report date range, Sample Period, and PQAO assignment
- Number required is based on the date range (number of full months or quarters)

Flow Rate Verifications (2)

- Number of Obs: Number of Flow type RP transactions submitted in the date range
- Average %D: Arithmetic mean of relative percent differences
- %Complete: 100 X Number of Obs / Number required

Flow Rate Verifications (3)

- Bias

$$Bias\_Estimate = \frac{1}{n} \bullet \sum_{i=1}^{n} |d_i| + t_{0.95,n-1} \bullet \frac{AS}{\sqrt{n}}$$

  - Where

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

Flow Rate Verifications (4)

- Sign of Bias
  - If the 25th percentile of the relative percent difference and 75 percentile are both negative, then the sign of the bias is negative.
  - If the 25th percentile and 75 percentile are both positive, then the sign of the bias is positive.
  - If the 25th percentile is negative and the 75 percentile is positive, then the sign of the bias is undetermined (+/-)

Semi Annual Flow Rate Audits (1)

- Every 6 months, audit the flow rate of the PM_{10}, $PM_{10-2.5}$ and $PM_{2.5}$ particulate analyzers.
- Report is organized by pollutant
- Detail data is presented by Monitor and summarized first by year then by PQAO.
- Monitor detail Begin and End dates are the intersection of report date range, Sample Period, and PQAO assignment
- Number required is based on the date range (number of six-month periods)

Semi Annual Flow Rate Audits (2)

- Number of Quarters with data: Number of calendar quarters in date range with Flow Audit RA transactioins
- % Completeness: 100 X number of quarters with data / number required
- Criteria Met: a) The number of required audits were performed, and b) if 2 audits are required, then they are between 5 and 7 months appart.
- Numer of Observations per Quarter: Number of Flow Audit RA transactions submitted in quarter
- Average %d: Arithmetic mean of %d

Semi Annual Flow Rate Audits (3)

- Confidence limits on the mean relative percent difference of the **Flow Rate Verifications**:
  - Upper 95% Confidence Limit = Mean + 1.96 * Standard_Deviation
  - Lower 95% Confidence Limit = Mean – 1.96 * Standard_Deviation
  - These are displayed only for summary rows (year and PQAO)
- The report also computes the percent of the **Flow Rate Audit** percent differences between the confidence limits on the **Flow Rate Verifications**

Collocated Audits: Collocation Detail (1)

- The report contains a detail section (monitor level) and a summary section (by year and PQAO)
- The report is organized by pollutant (e.g. PM 10)
- Only measurement values above the following will be consdiered valid: TSP: 20 ug/m^3, Pb: 0.02 ug/m^3, PM10 hi-vol: 15 ug/m^3, PM10 low-vol: 3 ug/m^3, PM2.5: 3ug/m^3, PM10-2.5: 3ug/m^3
- The POC provided on the detail section is for the primary monitor
- Monitor detail Begin and End dates are the intersection of report date range, Sample Period, and PQAO assignment
- The number required is based on every 12 days
- Values for both Lead 12128 and 14129 will be combined

Collocated Audits: Collocation Detail (2)

- "# Obs" is the number of precision pairs (either submitted as RP or RD transactions)
- "# Valid": This is the number of collocation pairs with concentrations above the thresholds provided above
- % Complete: 100 X #Obs / #Req (i.e. ignores validity)
- Coefficient of Variation: (precision estimate)

$$CV = \sqrt{\frac{n \bullet \sum_{i=1}^{n} d_i^2 - (\sum_{i=1}^{n} d_i)^2}{2n(n-1)}} \bullet \sqrt{\frac{n-1}{\chi^2_{0.1,n-1}}}$$

Collocated Audits: Collocation Summary (1)

- The summary section provides summaries by year and PQAO
- The report is organized by pollutant, year, and method
- Values for both Lead TSP parameters (12128 and 14129) will be combined.
- # Sites: Number of distinct sites reporting with that method.
- # Collocated Required: 15% of the sites for the pollutant must have collocated monitors
- #Actually Collocated: Number of collocated monitors actually reporting data in the date range

Collocated Audits: Collocation Summary (2)

- # Required Sites Collocated: 100 X Sites collocated / collocated sites requred
- # Required: Number of collocation audits (i.e. precision data pairs) based on number of collocated monitors and 1 in 12 collocated sampling schedule
- # Obs: Number of precision data pairs reported.
- # Valid Obs: Number of collocation pairs with concentrations above the threshold in table 4 (c) of Appendix A

Collocated Audits: Collocation Summary (3)

- % Complete: 100 X #Obs / #Req (i.e. ignores validity)
- Coefficient of Variation:

$$CV = \sqrt{\frac{n \bullet \sum_{i=1}^{n} d_i^2 - (\sum_{i=1}^{n} d_i)^2}{2n(n-1)}} \bullet \sqrt{\frac{n-1}{\chi^2_{0.1,n-1}}}$$

  - Note: Only valid collocated pairs will be used for the CV calculation.

Performance Evaluation Program (PEP): (1)

- The PEP is an independent assessment used to estimate the total measurement system bias
- The Report presents summaries by Pollutant and PQAO (monitor level detail is not presented)
- For completeness of PM, the report displays the number of sites, the number of PEP audits required, and the number of PEP audits collected.
- For completeness of Lead, the report displays the above and the number of Collocated PEP audits required and collected

Performance Evaluation Program (PEP): (2)

- Bias:

$$Bias\_Estimate = \frac{1}{n} \bullet \sum_{i=1}^{n} |d_i| + t_{0.95,n-1} \bullet \frac{AS}{\sqrt{n}}$$

  - Where

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

Performance Evaluation Program: (3)

- Confidence limits on the mean relative percent difference of the PEP audits (PM 2.5 only):
  - Upper 90% Confidence Limit

$$UpperLimit = \frac{1}{n} \bullet \sum_{i=1}^{n} d_i + t_{0.95,n} \bullet \frac{s}{\sqrt{n}}$$

  - Lower 90% Confidence Limit

$$LowerLimit = \frac{1}{n} \bullet \sum_{i=1}^{n} d_i + t_{0.95,n} \bullet \frac{s}{\sqrt{n}}$$

  - Where

$$s = \sqrt{\frac{\sum_{i=1}^{n} (d_i - Mean)^2}{n-1}}$$

Lead Analysis Audits (1)

- The lead analysis audits are an assessment of the bias of the analytical procedure (i.e. the procedure used by the analysis lab/agency)
- Three audit samples at each of two levels are requred each quarter
- The report is organized by PQAO and presents results by year and quarter
- % Complteness per quarter: 100 X Number of audit-level analyses / 6 (with no more than 3 per level counting toward total)

Lead Analysis Audits (2)

- The Lab Id on the report is the "Analysis Agency" for the monitor that is submitted on the RA transaction.
- Bias

$$Bias\_Estimate = \frac{1}{n} \bullet \sum_{i=1}^{n} | d_i | + t_{0.95,n-1} \bullet \frac{AS}{\sqrt{n}}$$

  - Where

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

Questions?