Data Uncertainty and Data Quality Objectives

2019 EPA REGION 4 QUALITY ASSURANCE TRAINING

Lesson Goals
Understanding the concepts of:

DQOs

- **Project Level**
- Big Picture
- Full sets of specifications needed to design a data collection effort

Data Quality Objectives

DQIs

- **Data Set Level**
- Quantitative and qualitative characteristics associated with the data

Data Quality Indicators

MQOs

- **Measurement Level**
- Acceptance criteria for individual DQIs

Measurement Quality Objectives

Data Quality Objectives (DQOs)

Specifications needed to determine the type, quantity, and quality of data needed to reach defensible decisions or make credible estimates

- Criteria Pollutant DQOs-40 CFR Part 58 Appendix A Section 2.3.1
- DQOs answer the following questions:
  - Why are data needed?
  - What measurements are required?
  - What do they need to represent?
  - How will the data be used?
  - How much uncertainty can be tolerated?

The DQOs in CFR are **goals.**

If the goals are not achieved decisions are made with less certainty

What is the DQO Process?

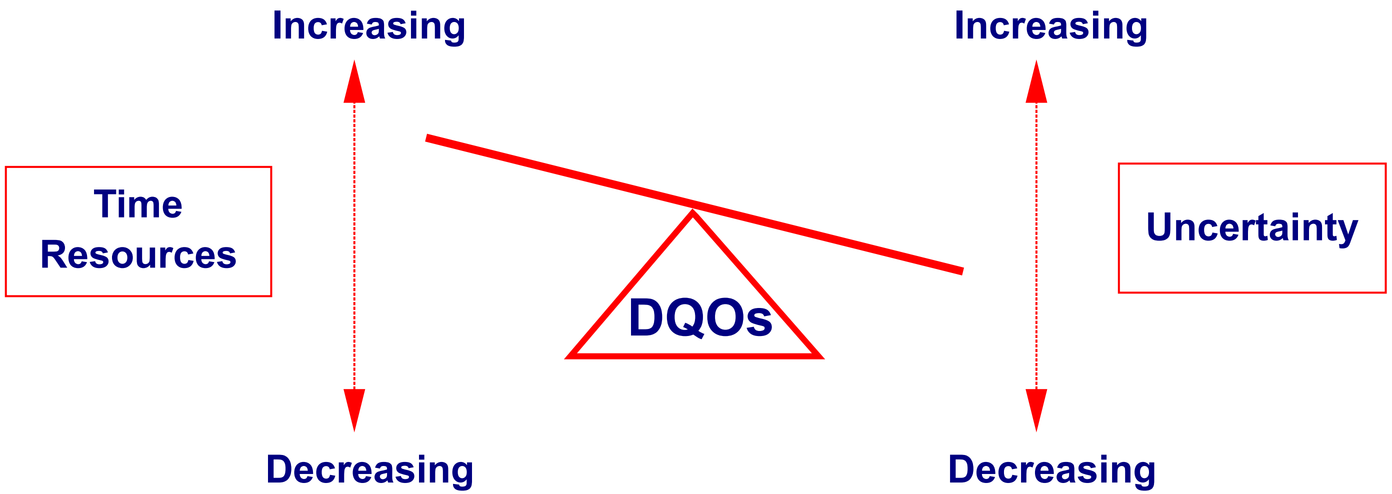
A systematic planning process for generating environmental data that will be sufficient for their intended use (decision).

Who makes the decision(s)?

- Manager
- Director
- Commissioner
- Cabinet Secretary
- **Governor**
- **EPA**

DQO Process: Underlying Principles

1. All collected data have error
2. Nobody can afford absolute certainty
3. The DQO Process defines tolerable error rates
4. Absent DQOs, decisions are uninformed
5. Uninformed decisions tend to be conservative and expensive



Systematic/Scientific DQO Planning

Designed to answer:

What do you need?

Why do you need it?

How will you use it?

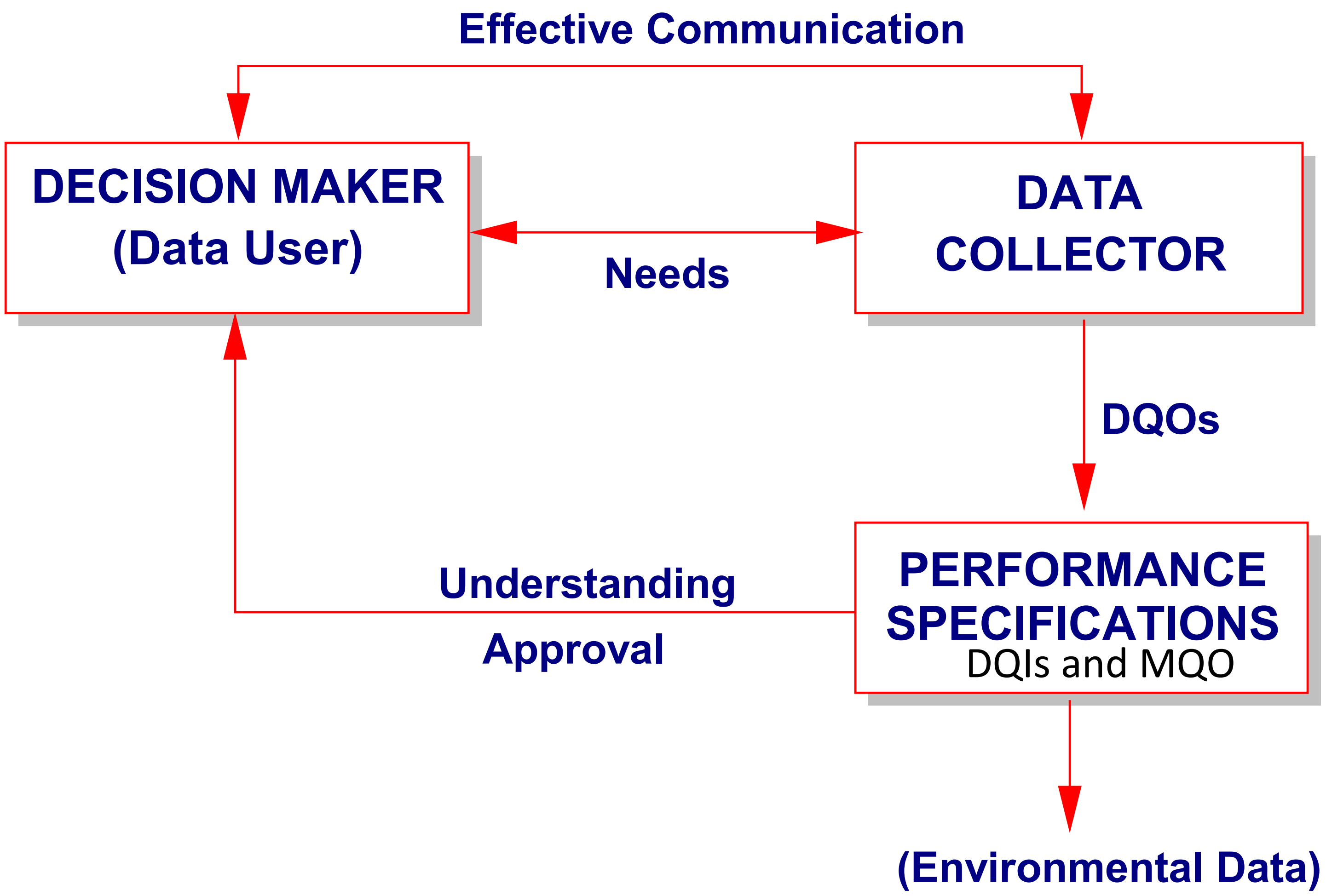
What is your tolerance for errors?

7-Step DQO Process:

1. State the problem to be resolved
2. Identify the decision to be made
3. Identify the inputs to the decision
4. Define the boundaries
5. Develop a decision rule
6. Specify the tolerable limits on decision errors
7. Optimize the design for obtaining the data

See Guidance on the Systematic Planning using the DQO Process
https://www.epa.gov/quality/agency-wide-quality-system-documents

A Quality Planning Model



Decision Errors:
Synonyms and Plain English

If the baseline assumption is that the site is ***greater than*** the action limit (e.g., non-attainment) , then:

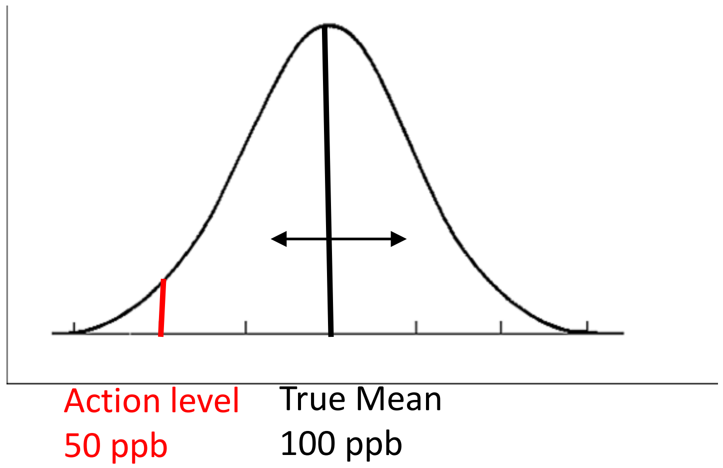
False Rejection Error F(r), Type I Error, False Positive

- Deciding the site is in attainment when it is not
- A missed opportunity for correction
- Allowing a hazard to public health or the ecosystem

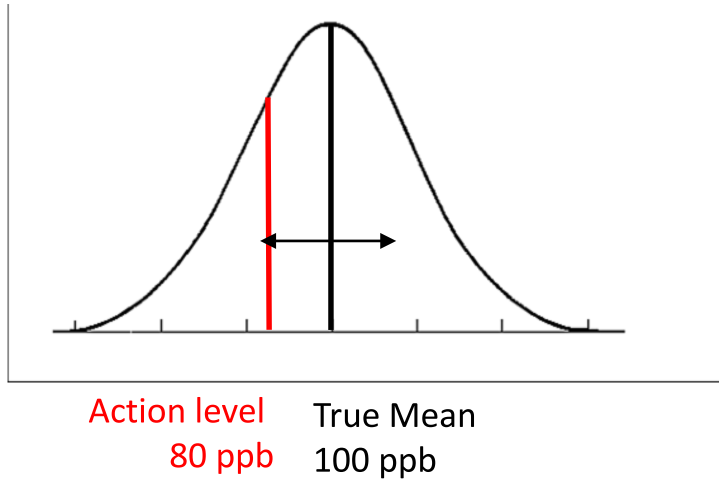
False Acceptance Error F(a), Type II Error, False Negative

- Deciding the site is not in attainment when it is
- An overreaction to a situation
- Wasted resources, unnecessary expenditure

The Probability of Making Decision Errors



If the true mean is much greater than the action level, few low readings will occur. So, there is a less chance of making a decision error.



If the true mean is close to the action level, many low readings will occur. Decision errors are much more likely.

Tolerable Decision Error Limits

Regulatory Language

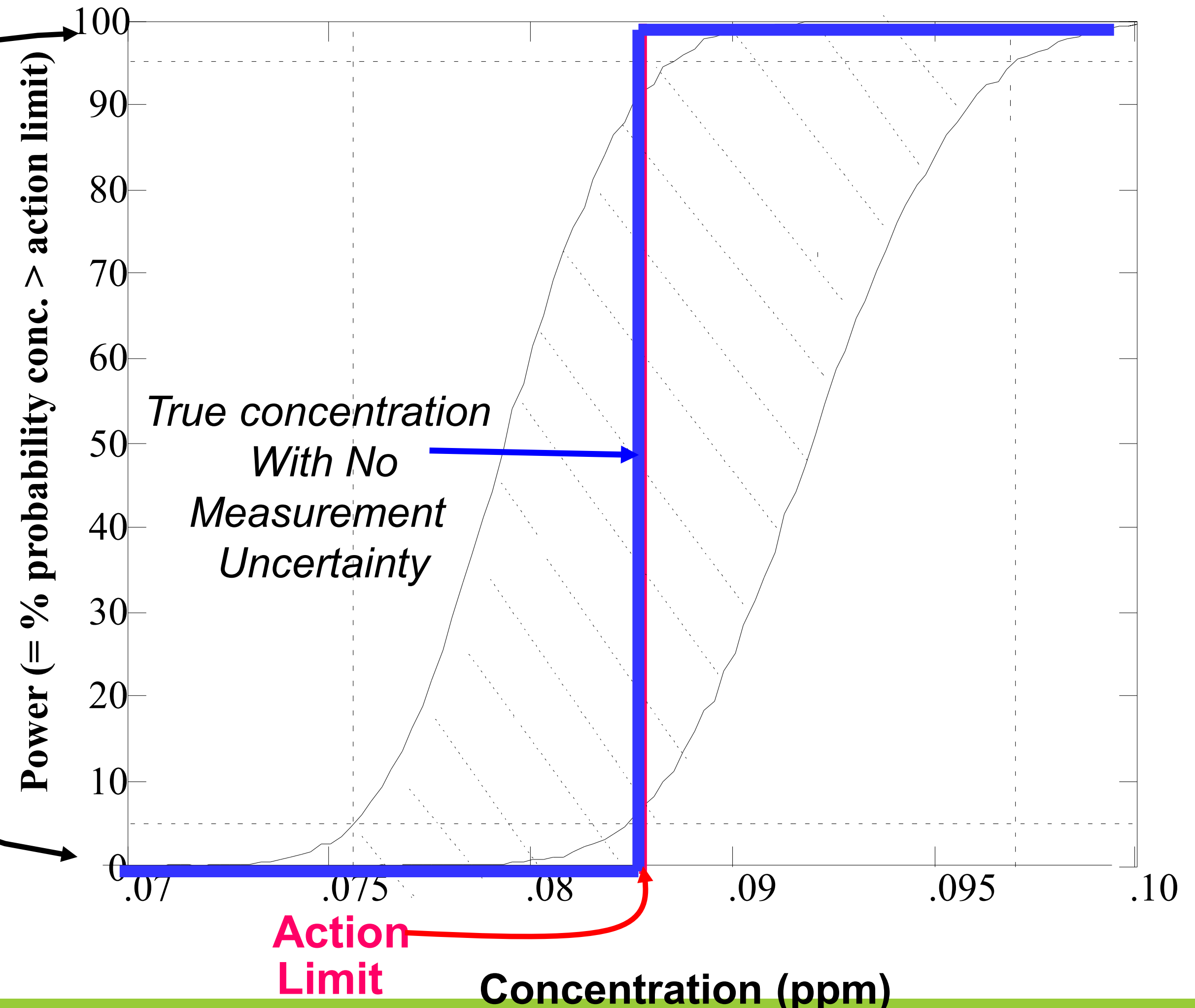
§2.3.1.2 *Measurement Uncertainty for Automated O_3 Methods.* The goal for acceptable measurement uncertainty is defined for precision as an upper 90 percent confidence limit for the CV of 7 percent and for bias as an upper 95 percent confidence limit for the absolute bias of 7 percent.

Ozone Performance Curve
(NAAQS prior to 2008 Change)

Baseline Condition 3-year 4th highest max mean conc. > action limit

Decision error limits

The probability of making a decision error



Ozone Performance Curve
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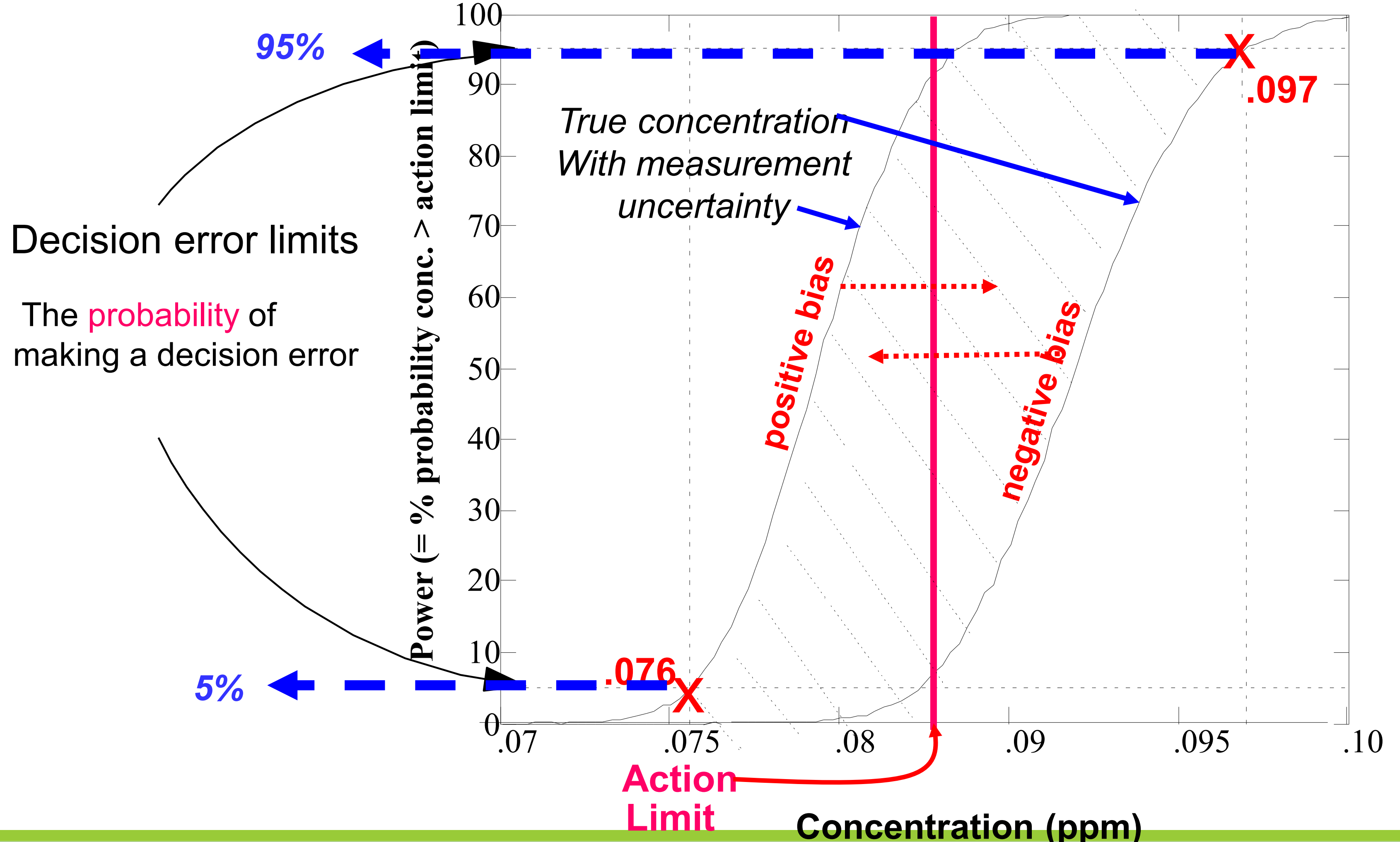


With 7% negative bias and
7% imprecision, an ozone site with A 3 year 4th highest max value of 0.097ppm has a 95% probability of being classified above the action limit (NAAQS)

With 7% positive bias and
7% imprecision, an ozone site with a 3 year 4th highest max value of 0.076 ppm has a 5% probability of being classified above the action limit (NAAQS)

Plain Language (for ozone)

If you have a design value that is ≤ 75 ppb (attainment) or ≥ 97 ppb (non-attainment) and precision and bias that meet the DQOs, then you will make the correct attainment decision 95% of the time

For design values between 75 ppb and 97 ppb even if the precision and bias meets the DQOs, chances of making the correct attainment decision diminish as the design value gets closer to the action limit.

The Quantitative DQOs (40 CFR Part 58 App A)

§2.3.1.1 $PM_{2.5}$ – 10% CV $\pm$ 10% Bias

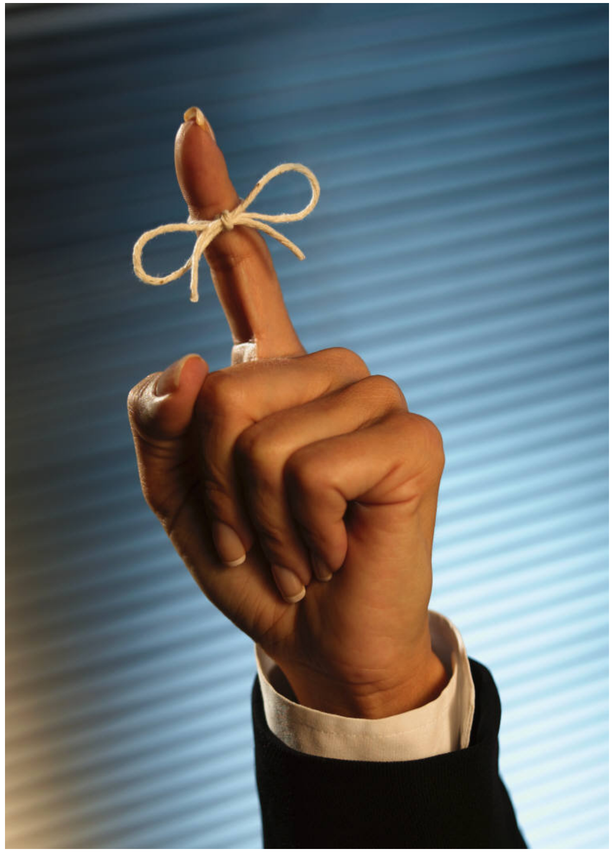
§2.3.1.2 Ozone – 7% CV $\pm$ 7% Bias

§2.3.1.3 Lead – 20% CV $\pm$ 15% Bias

§2.3.1.4 NO_2 – 15% CV $\pm$ 15% Bias

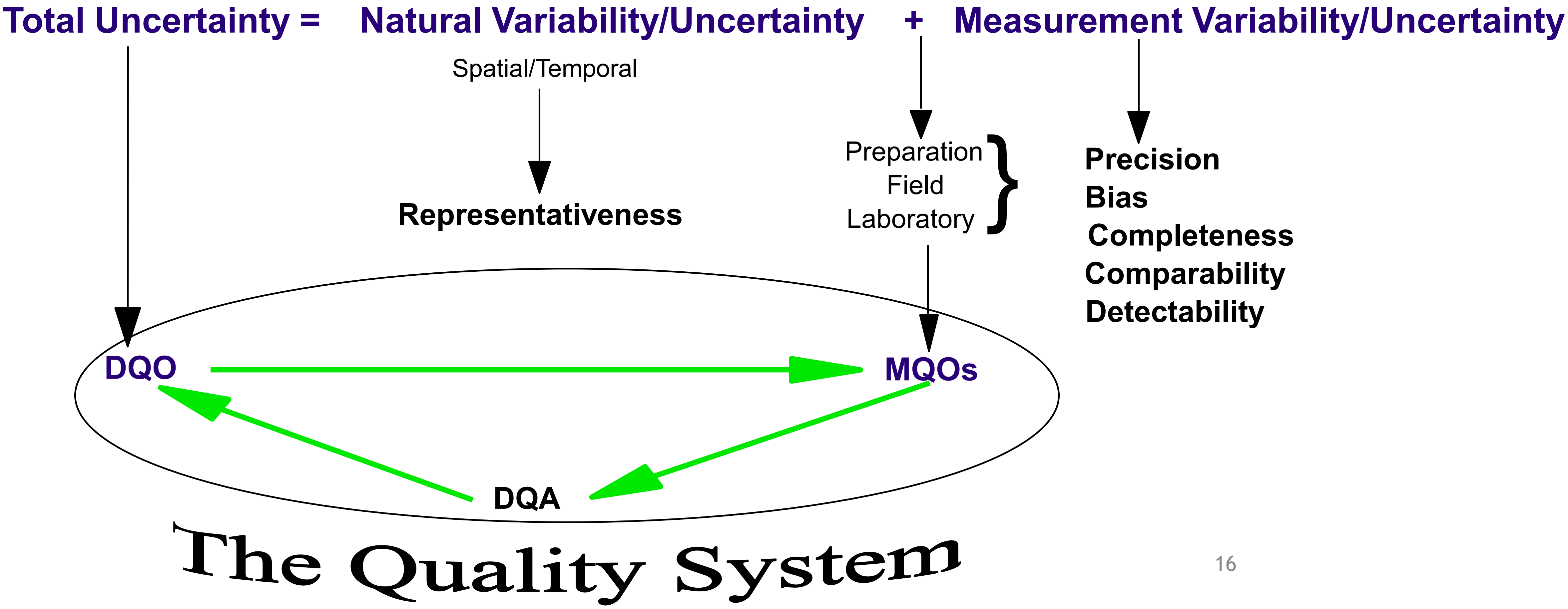
§2.3.1.5 SO_2 – 10% CV $\pm$ 10% Bias

CO - 10% $\pm$ 10% Bias



EPA started providing quantitative DQOs in 1997 ($PM_{2.5}$) and as a NAAQS comes up for review

DQO Goal--- Understanding and Controlling Uncertainty to Acceptable Levels for Informed Decision Making



Data Quality Indicators (DQIs)

Are quantitative and qualitative attributes or characteristics associated with data

The principal DQIs:

- Representativeness
- Precision
- Bias
- Completeness
- Comparability
- Sensitivity

Representativeness

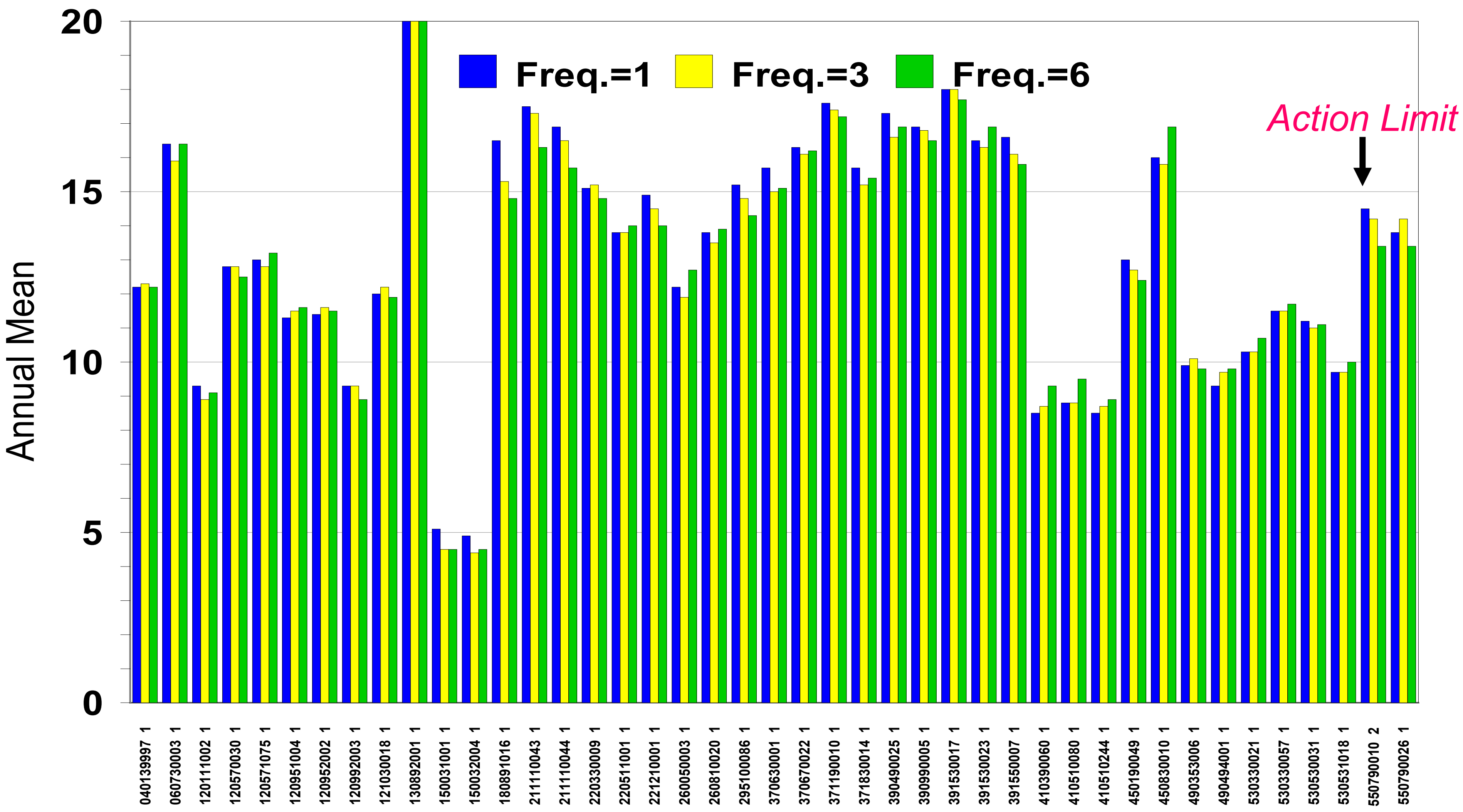
Refers to the measure of the degree to which data suitably represent a characteristic of a population, parameter variations at a sampling point, a process condition, or an environmental condition

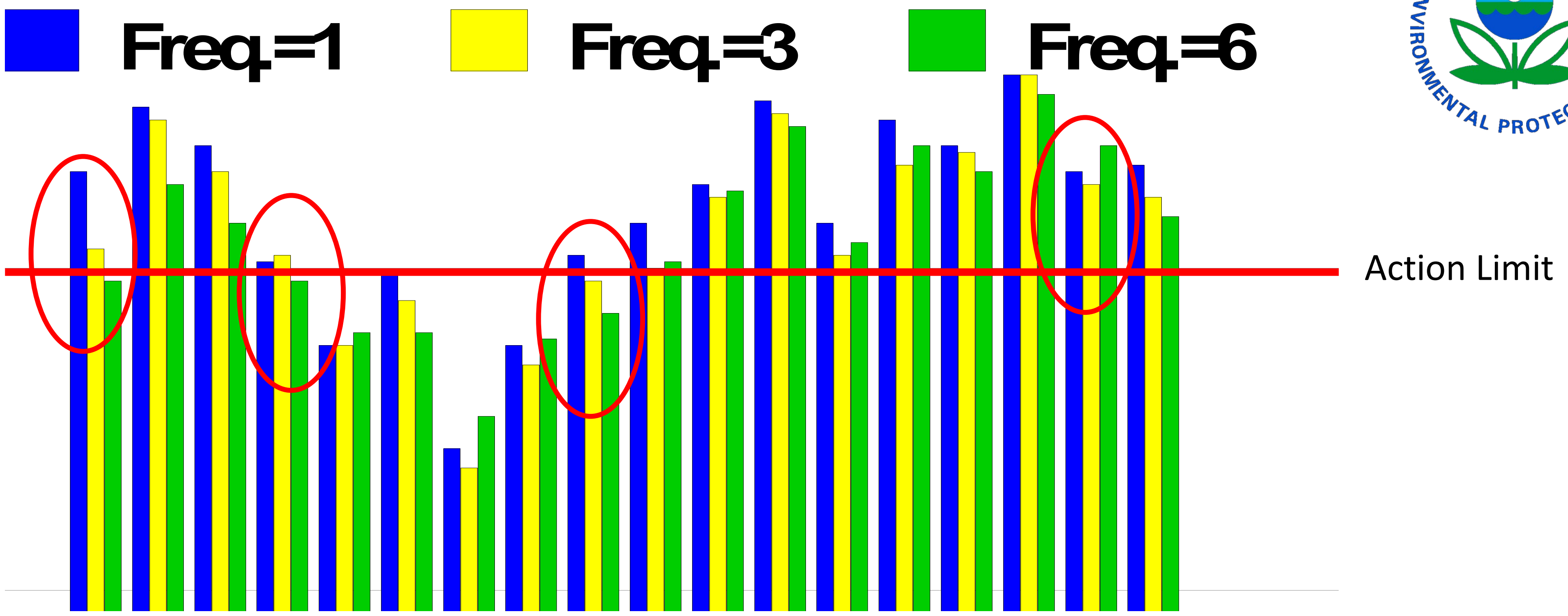
- *Concentration of air for the spatial scale of interest*

It does not matter how precise or unbiased the measurement values are if a site is unrepresentative of the population it is presumed to represent!

Temporal Representativeness of PM2.5 Sampling

Comparing Annual Means from Every Day sampling to those calculated from 1-in-3 and 1-in-6 frequencies. Only complete sites included.





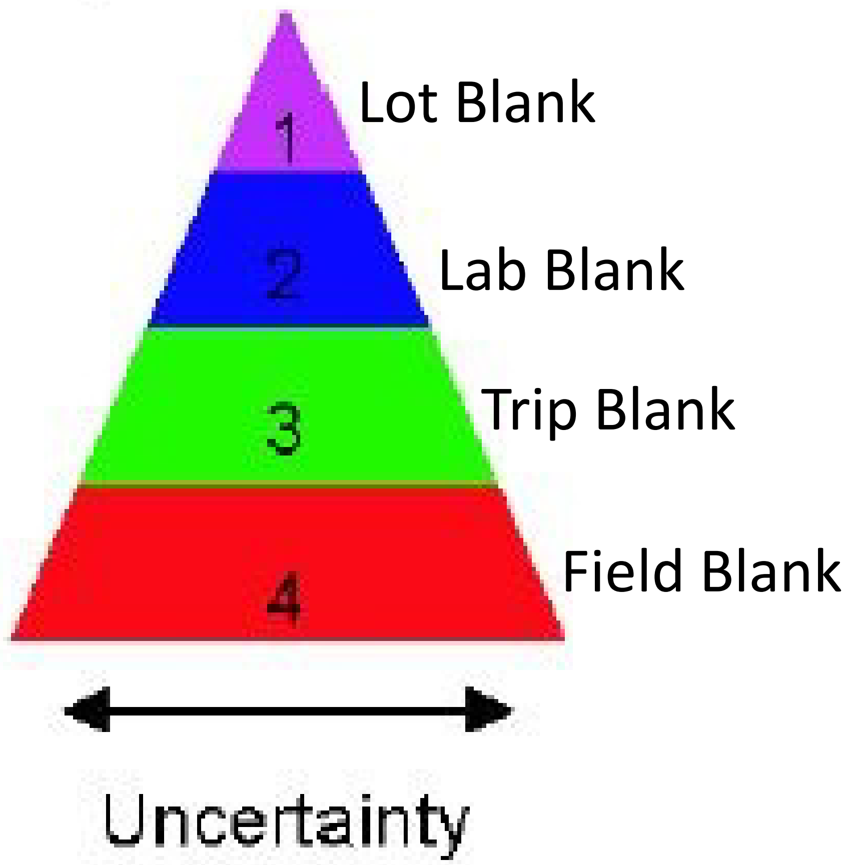
Temporal variability can affect attainment decisions

Every day sampling does not always provide the highest mean conc., but does provide the user with more confidence in the annual estimate.

Measurement Uncertainty

A term used to describe deviations from a true concentration or estimate that are related to the **measurement process** and not to spatial or temporal variability of the air being measured.

Can be an overall assessment of measurement uncertainty or an assessment at various measurement phases



Precision

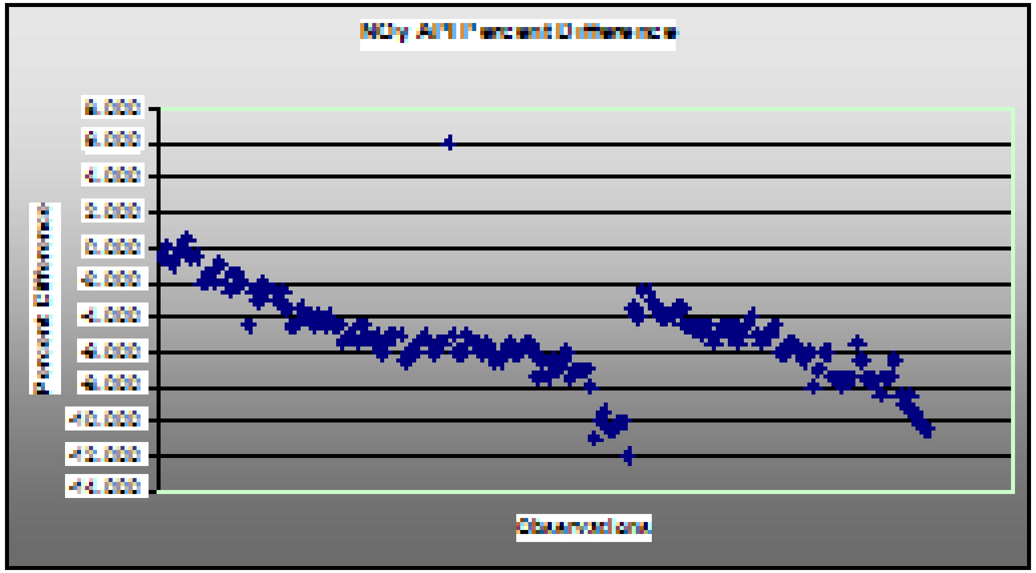
A measure of agreement among repeated measurements of the same property under identical, or substantially similar, conditions.

Bias

A systematic or persistent distortion of a measurement process that causes error in one direction

A bias DQI is a quantitative indicator of the magnitude of systematic error resulting from:

- biased sampling design
- calibration errors
- unaccounted-for interferences
- chronic sample contamination



Accuracy

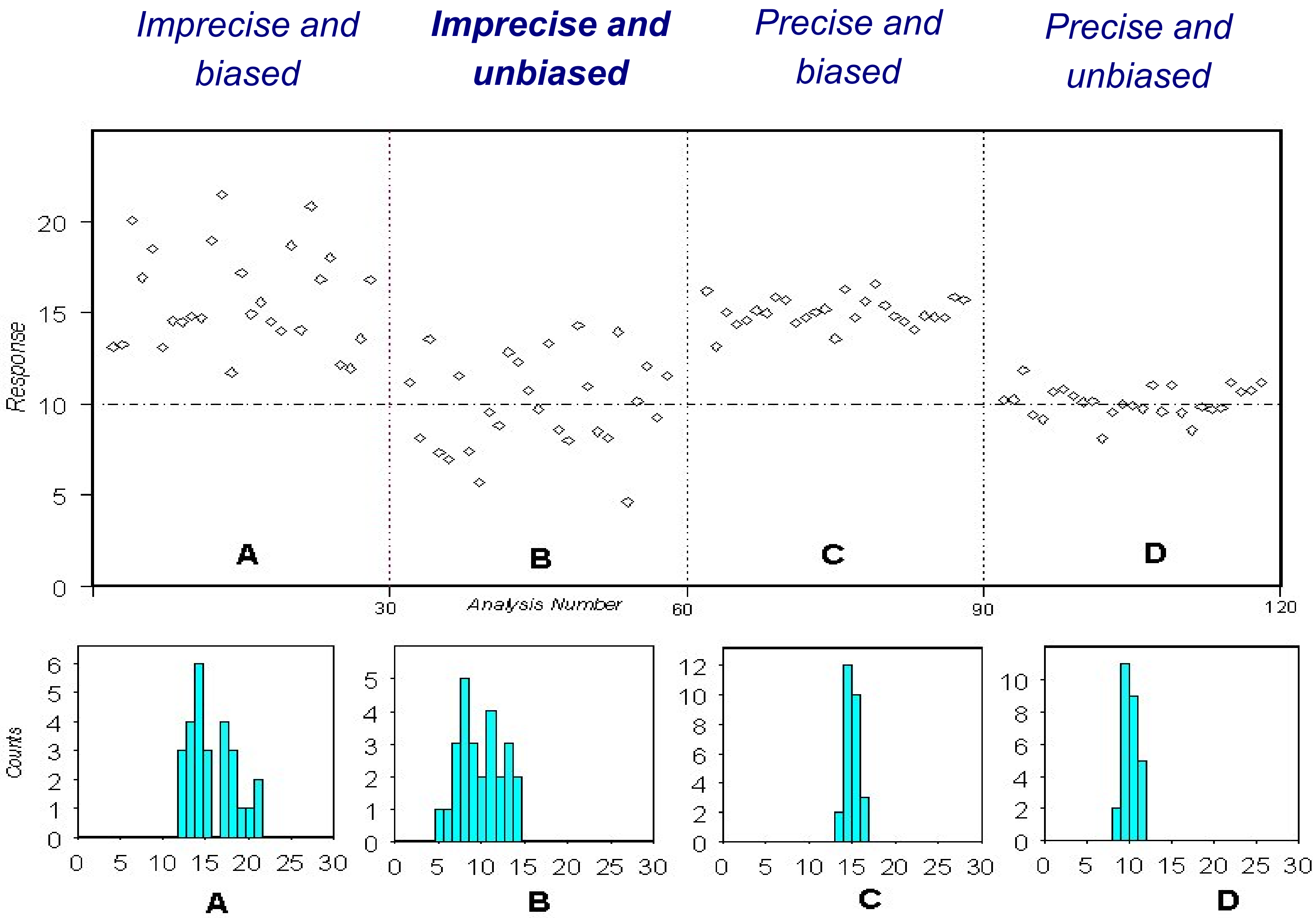
A measure of the overall agreement of a measurement to a known value

- when random errors are tightly controlled, bias dominates the overall accuracy
- when random errors predominate, variance dominates the overall accuracy

- Accuracy is composed of precision and bias

- EPA policy suggests using bias and precision as separate measures rather than accuracy

Influence of Bias and Imprecision on Overall Accuracy



The DASC Tool Provides the DQO Statistics

CV_{ub} (%)		Bias (%)	
n	S_d	S_{d2}	$\Sigma\|d\|$
500	2.633	15.148	1012.937
n-1	Σd	Σd^2	$\Sigma\|d\|^2$
499	-446.201	3858.540	3858.540

"AB" (Eqn 4)	2.026
"AS" (Eqn 5)	1.903

Bias (%) (Eqn 3)	2.17
Both Signs Positive	FALSE
Signed Bias (%)	+/-2.17
Both Signs Negative	FALSE
CV (%) (Eqn 2)	2.75
Upper Probability Limit	4.27
Lower Probability Limit	-6.05

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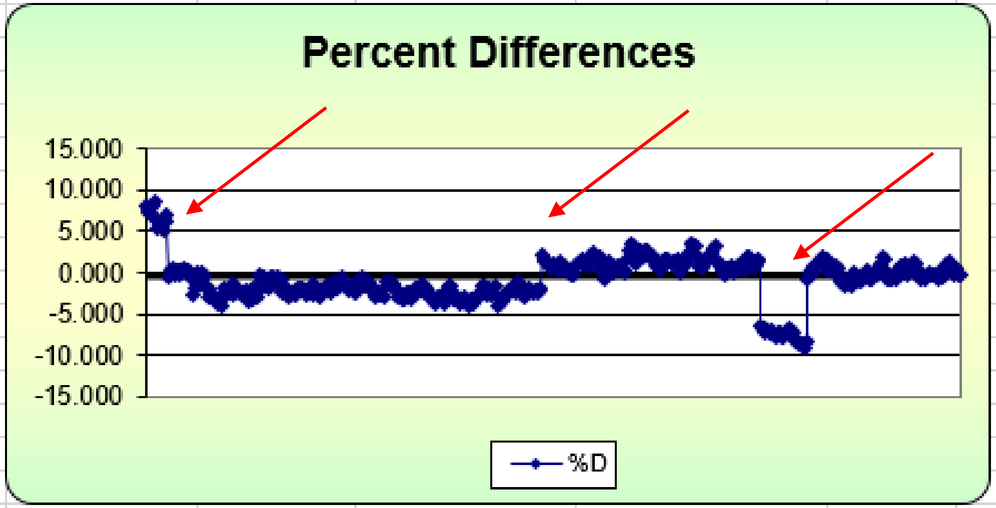
Print Worksheet



O_3 Assessments

Site ID: {Enter Site ID}		Pollutant type: O_3					CV_{ub} (%)
Meas Val (Y)	Audit Val (X)	d (Eqn. 1)	25th Percentile	d^2	|d|	$\|d\|^2$	
75.7	70	8.143	-2.300	66.306	8.143	66.306	
75	70	7.143	75th Percentile	51.020	7.143	51.020	
75.2	70	7.429	0.677	55.184	7.429	55.184	
75	70	7.143		51.020	7.143	51.020	
75.7	70	8.143		66.306	8.143	66.306	
76	70	8.571		73.469	8.571	73.469	
74.5	70	6.429		41.327	6.429	41.327	
73.7	70	5.286		27.939	5.286	27.939	
74.2	70	6.000		36.000	6.000	36.000	
73.9	70	5.571		31.041	5.571	31.041	
73.9	70	5.571		31.041	5.571	31.041	
73.5	70	5.000		25.000	5.000	25.000	
74.8	70	6.857		47.020	6.857	47.020	
74.4	70	6.286		39.510	6.286	39.510	
73.5	73.9	-0.541		0.293	0.541	0.293	
74	73.9	0.135		0.018	0.135	0.018	
74.3	73.9	0.541		0.293	0.541	0.293	
73.8	73.9	-0.135		0.018	0.135	0.018	
73.7	73.9	-0.271		0.073	0.271	0.073	
74.1	73.9	0.271		0.073	0.271	0.073	
74.1	73.9	0.271		0.073	0.271	0.073	
73.7	73.9	-0.271		0.073	0.271	0.073	
74	73.9	0.135		0.018	0.135	0.018	
74.1	73.9	0.271		0.073	0.271	0.073	
74.2	73.9	0.406		0.165	0.406	0.165	
74.1	73.9	0.271		0.073	0.271	0.073	
74	73.9	0.135		0.018	0.135	0.018	
73.5	73.9	-0.541		0.293	0.541	0.293	
73.4	73.9	-0.677		0.458	0.677	0.458	
72	73.9	-2.571		6.610	2.571	6.610	
72.5	73.9	-1.894		3.589	1.894	3.589	
72.6	73.9	-1.759		3.095	1.759	3.095	
73.9	73.9	0.000		0.000	0.000	0.000	
73.3	73.9	-0.812		0.659	0.812	0.659	
73.8	73.9	-0.135		0.018	0.135	0.018	
73.7	73.9	-0.271		0.073	0.271	0.073	
73.4	73.9	-0.677		0.458	0.677	0.458	
72.4	73.9	-2.030		4.120	2.030	4.120	
72.4	73.9	-2.030		4.120	2.030	4.120	

n	S_d	S_{d2}
500	2.633	15.1
n-1	Σd	Σd^2
499	-446.201	3858.5

CV (%) (Eqn 2)	2.75
Upper Probability Limit	4.27

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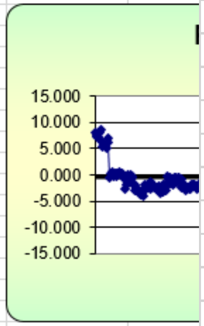


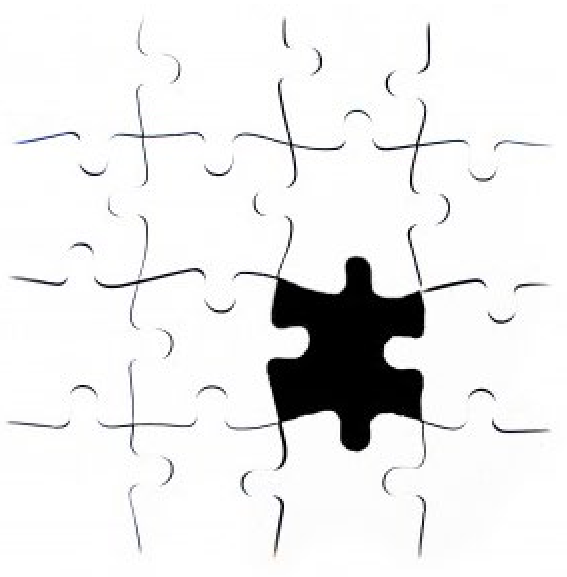
Comparability

- Is a measure of the confidence with which one data set or method can be compared to another
- Comparability of datasets is critical to evaluating their measurement uncertainty and usefulness
- Criteria pollutant quality indicator summary reports can help to assess data comparability among monitoring sites in a PQAO
- National Performance Evaluation Programs (NPEP) evaluate data comparability among PQAOs

Completeness

A measure of the amount of valid data obtained from a measurement system, expressed as a percentage of the number of valid measurements that should have been collected

- the DQI for completeness is often expressed as a percentage



*Defined in 40 CFR Part 50 for the individual NAAQS pollutants

Sensitivity- Detection Limits

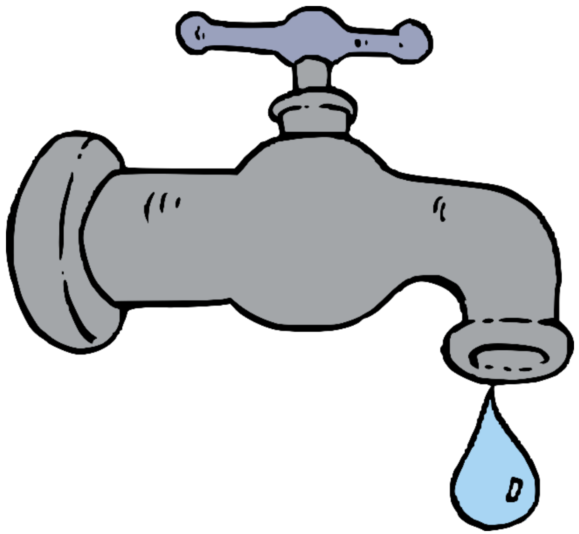
Is the capability of a method or instrument to discriminate between measurement responses representing different levels of the variable of interest

- Sensitivity can be regarded as detection limit
  - but this term is often used without defining what is intended (minimum detection or quantitation)
- A sensitivity DQI describes the capability of measuring a constituent at low levels
- Federal reference and equivalent methods meet sensitivity requirements if operated properly
- Methods requiring laboratory analysis define the sensitivity of the methods and instruments used in the analysis
- Monitoring organization should run a method detection limit (MDL) for their monitoring and laboratory instruments.

MDLs Per 40 CFR Part 136 Appendix B

The *method detection limit* (MDL) is defined as the minimum concentration of a substance that can be measured and reported with 99% confidence that the analyte concentration is greater than zero and is determined from analysis of a sample in a given matrix containing the analyte.

- Initially designated for water analyses, but adapted for many other matrices.
- Ambient air embraces the MDL Method Update Rule (MUR) 40 CFR Part 136 Appendix B.



Measurement Quality Objectives (MQOs)

- DQOs drive the MQOs
- MQOs are the acceptance or performance criteria for individual DQIs
- Can be performance criteria for overall measurement uncertainty or a criteria for an measurement phase (i.e., preparation, transportation, laboratory, field)

DQOs vs MQOs

DECISION MAKER

DQOs: Big picture

- Aggregate of all QC checks collected at site and across pollutant network
- CV computation and confidence limits
- Indicator of systemic issues
  - If DQOs not achieved big picture questions & investigation needed.
  - For example, warning limits may need to be tightened or aged monitors replaced

DATA COLLECTOR

MQOs: Individual Analyzer

- Single QC checks
- Percent difference or difference computation
- Assess how well the analyzer compares to the standard against which it was challenged – at that moment in time
  - If fails, investigation needed to determine cause of the exceedance, in order to return the analyzer to an "in control status.

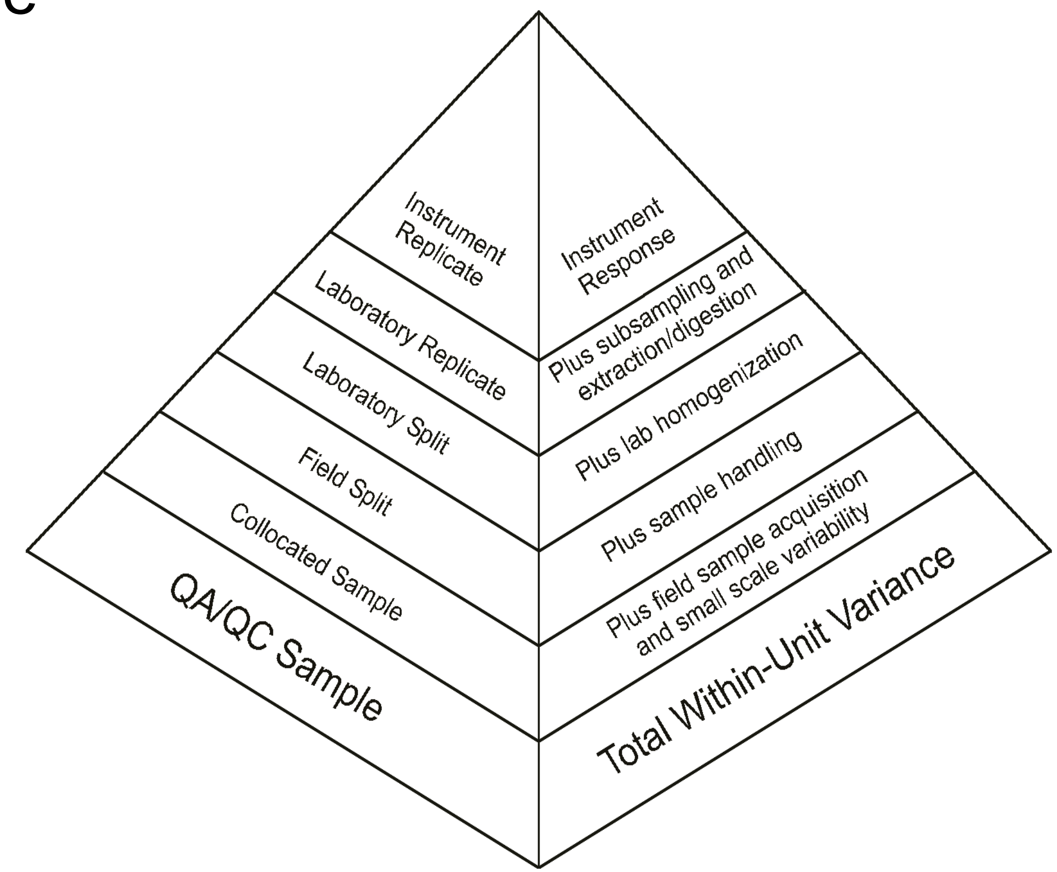
Where do MQOs come from?

- Regulatory requirements
- Analytical Methods
- Technical Experience
- Derived from the project designed process and specified by the Project Planning Team

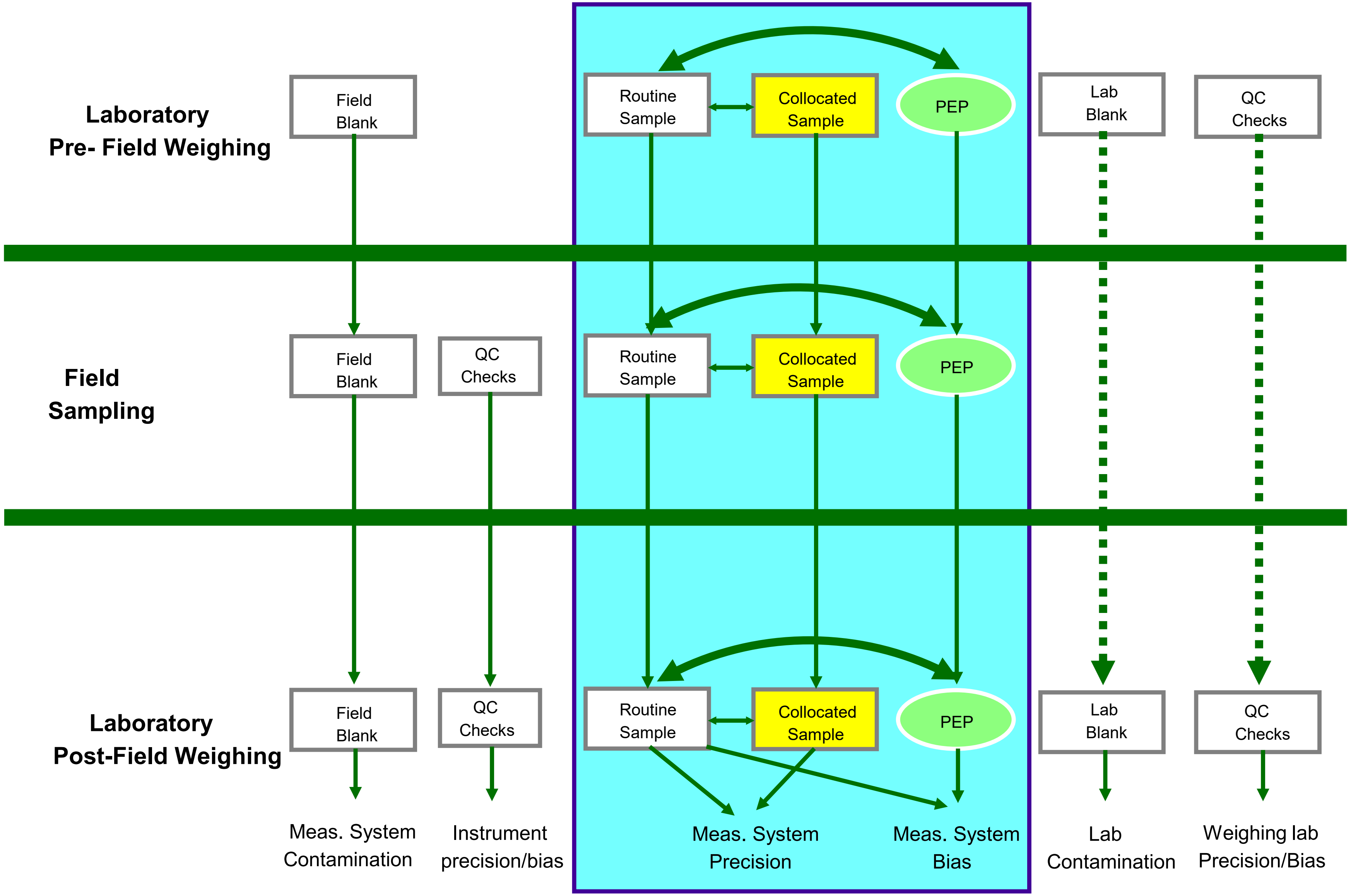
Establishing MQOs

Decomposing total study variance facilitates the identification of the relative importance of components of total error

- this exercise helps determine what kind of QC samples to employ
- MQOs on specific measurement components must reflect the requirements for total measurement error
- Individual Measurement Quality Objectives (MQOs) should be established for components of variance that primarily drive the total variability



PM2.5 Quality Control Sampling Scheme-MQOs



Various QC checks included in data collection activity to assess and control measurement phases so that overall quality is acceptable

Examples of MQOs

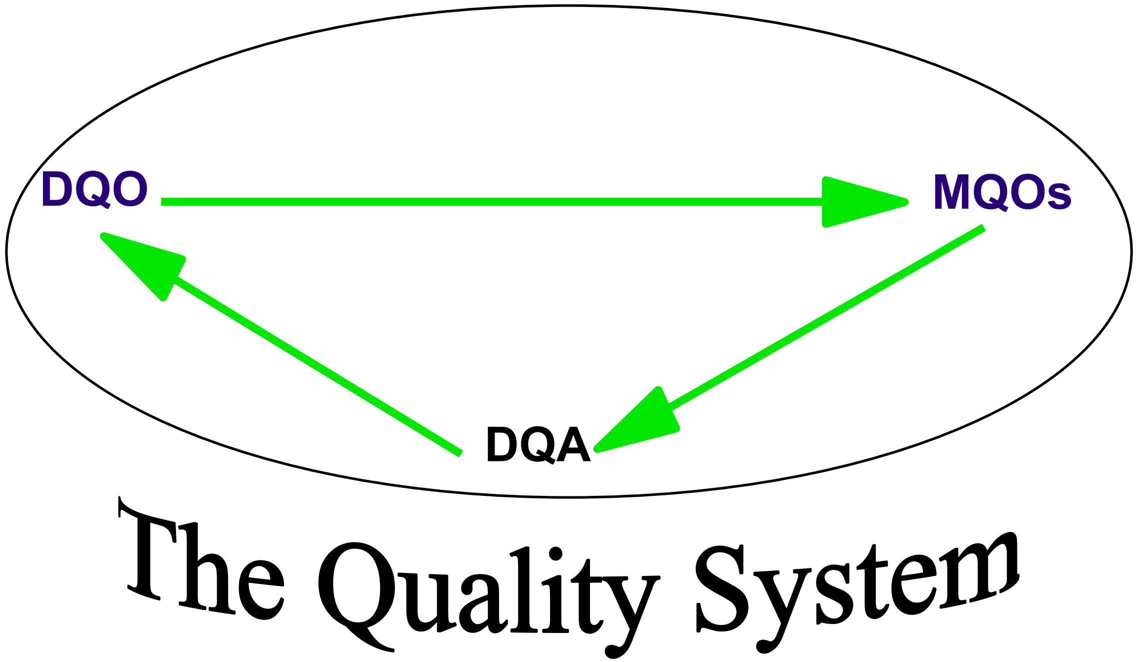
Monitoring Org Implementation

- Samples (PM and Pb)
  - Collocation - (Meas. System Precision)
  - Field/Trip/Lab Blanks –
  - Routine sample reweighs (replicates)
- Verifications
  - Flow/Temp/Pressure (PM & Pb)
  - Zero/Span/Precision (Gaseous)
- Audits (Independent within Monitoring Org)
  - Flow Rate (PM & Pb)
  - Annual Performance Evaluations (Gaseous)
- Yearly Calibrations
- Standards Recertifications

Acceptance criteria for MQOs found in Validation Templates in the QA Handbook and discussed in Lesson 6

Completing the Quality System Circle

- The DQO process provides the level of uncertainty that can be tolerated by the decision maker(s)
- That uncertainty is used to determine the number of samples to take and the MQOs needed to meet to DQO
- Data quality assessments (DQA) are performed to determine if DQOs have been met or corrective actions are need to bring the measurements into acceptable quality **<u>or</u>** if the quality cannot be attained whether the DQOs need to be revised (EPA decision).



Data Uncertainty and Data Quality Objectives

Questions? Comments? Concerns?

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