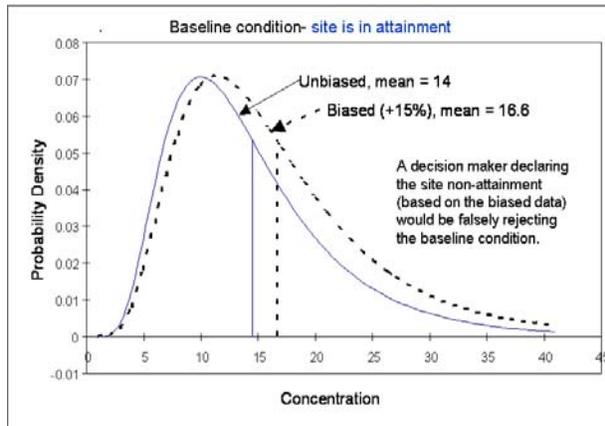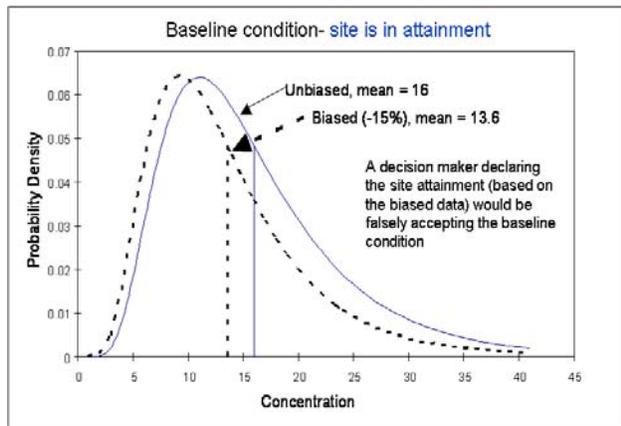# 3.0 Data Quality Objectives

Data collected for the Ambient Air Quality Monitoring Program are used to make very specific decisions that can have an economic impact on the area represented by the data. Data quality objectives (DQOs) are qualitative and quantitative statements derived from the DQO Planning Process that clarify the purpose of the study, define the most appropriate type of information to collect, determine the most appropriate conditions from which to collect that information, and specify tolerable levels of potential decision errors. Throughout this document, the term *decision maker* is used. This term represents individuals that are the ultimate users of ambient air data and therefore may be responsible for setting the NAAQS (or other objective), developing a quality system, or evaluating the data (e.g., NAAQS comparison). The DQO will be based on the data requirements of the decision maker who needs to feel confident that the data used to make environmental decisions are of adequate quality. The data used in these decisions are never error free and always contain some level of uncertainty. Because of these uncertainties or errors, there is a possibility that decision makers may declare an area "nonattainment" when the area is actually in "attainment" (Fig. 3.1 a false rejection of the baseline condition) or "attainment" when actually the area is in "nonattainment" (Fig. 3.2 false acceptance of the baseline condition)[1]. Figures 3.1 and 3.2 illustrate how false rejection and acceptance errors can affect a NAAQS decision based on an annual mean concentration value of 15 and the baseline condition that the area is in attainment. There are serious political, economic and health consequences of making such decision errors. Therefore, decision makers need to understand and set limits on the probabilities of making incorrect decisions with these data.

Figure 3.1 Effect of positive bias on the annual average estimate, resulting in a false rejection error.

Figure 3.2 Effect of negative bias on the annual average resulting in a false acceptance error.

In order to set probability limits on decision errors, one needs to understand and control uncertainty. Uncertainty is used as a generic term to describe the sum of all sources of error associated with an EDO and can be illustrated as follows:

$$S_o^2 = S_p^2 + S_m^2 \qquad\qquad \textit{Equation 3-1}$$

where:

S_o = overall uncertainty
S_p = population uncertainty (spatial and temporal)
S_m = measurement uncertainty (data collection).

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[1] "Guidance on Systematic Planning Using the Data Quality Objectives Process," EPA QA/G-4 U.S. Environmental Protection Agency, QAD, February 2006. http://www.epa.gov/quality1/qs-docs/g4-final.pdf

The estimate of overall uncertainty is an important component in the DQO process. Both population and measurement uncertainties must be understood.

Population uncertainties - The most important data quality indicator of any ambient air monitoring network is representativeness[2]. This term refers to the degree to which data accurately and precisely represent a characteristic of a population, a parameter variation at a sampling point, a process condition, or a condition. Population uncertainty, the spatial and temporal components of error, can affect representativeness. These uncertainties can be controlled through the selection of appropriate boundary conditions (the monitoring area and the sampling time period/frequency of sampling) to which the decision will apply, and the development of a proper statistical sampling design (see Section 6). Appendix B of the Quality Staff's document titled *Guidance for Quality Assurance Project Plans (EPA/G5)[3]* provides a very good dissertation on representativeness. 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. Assuring the collection of a representative air quality sample depends on the following factors:

- selecting a network size that is consistent with the monitoring objectives and locating representative sampling sites;
- identifying the constraints on the sampling sites that are imposed by meteorology, local topography, emission sources, land access and the physical constraints and documenting these; and
- selecting sampling schedules and frequencies that are consistent with the monitoring objectives.

Measurement uncertainties are the errors associated with the EDO, including errors associated with the field, preparation and laboratory measurement phases. At each measurement phase, errors can occur, that in most cases, are additive. The goal of a QA program is to control measurement uncertainty to an acceptable level through the use of various quality control and evaluation techniques. In a resource constrained environment, it is most important to be able to calculate and evaluate the total measurement system uncertainty (S_m) and compare this to the DQO. If resources are available, it may be possible to evaluate various phases (e.g., field, laboratory) of the measurement system.

Three data quality indicators are most important in determining total measurement uncertainty:

- **Precision** - a measure of agreement among repeated measurements of the same property under identical, or substantially similar, conditions. This is the random component of error. Precision is estimated by various statistical techniques typically using some derivation of the standard deviation.

- **Bias** - the systematic or persistent distortion of a measurement process which causes error in one direction. Bias will be determined by estimating the positive and negative deviation from the true value as a percentage of the true value.

- **Detection Limit** - The lowest concentration or amount of the target analyte that can be determined to be different from zero by a single measurement at a stated level of probability. Due to the fact the NCore sites will require instruments to quantify at lower concentrations, detection limits are becoming more important. Some of the more recent guidance documents suggest that monitoring organizations develop method detection limits (MDLs) for continuous instruments and or analytical methods. Many monitoring organizations use the default MDL listed in AQS for a particular method. These default MDLs come from instrument vendor advertisements and/or

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[2] http://www.epa.gov/quality1/glossary.htm#R
[3] http://www.epa.gov/quality1/qa_docs.html

method manuals. Monitoring organizations should not rely on instrument vendor's documentation on detection limits but determine the detection limits that are being achieved in the field during routine operations. Use of MDL have been listed in the NCore Precursor Gas Technical Assistance Document (TAD)[4].

Accuracy is a measure of the overall agreement of a measurement to a known value and includes a combination of random error (precision) and systematic error (bias) components of both sampling and analytical operations. This term has been used throughout the CFR and in some sections of this document. Whenever possible, it is recommended that an attempt be made to distinguish measurement uncertainties into precision and bias components. In cases where such a distinction is not possible, the term accuracy can be used.

Other indicators that are considered during the DQO process include **completeness** and **comparability**. Completeness describes the amount of valid data obtained from a measurement system compared to the amount that was expected to be obtained under correct, normal conditions. For example, a $PM_{2.5}$ monitor that is designated to sample every sixth day would be expected to have an overall sampling frequency of one out of every six days. If, in a thirty day period, the sampler misses one sample, the completeness would be recorded as four out of five, or 80 percent. Data completeness requirements are included in the reference methods (40 CFR Part 50). Comparability is a measure of the confidence with which one data set or method can be compared to another, considering the units of measurement and applicability to standard statistical techniques. Comparability of datasets is critical to evaluating their measurement uncertainty and usefulness.

Performance Based Measurement System Concept: Consistency vs. Comparability

The NATTS Program proposes to use of the performance based measurement system (PBMS) concept. In simple terms, this means that as long as the quality of data that the program requires (DQOs) are defined, the data quality indicators are identified, and the appropriate measurement quality objectives (MQOs) that quantify that the data quality are met, any sampling/analytical method that meets these data quality requirements should be appropriate to use in the program. The idea behind PBMS is that if the methods meet the data quality acceptance criteria the data are "comparable" and can be used in the program. Previous discussions in this document allude to the need for "nationally consistent data", "utilization of standard monitoring methods" and "consistency in laboratory methods". Comparability is a data quality indicator because one can quantify a number of data quality indicators (precision, bias, detectability) and determine whether two methods are comparable. Consistency is not a data quality indicator and requiring that a particular method be used for the sake of consistency does not assure that the data collected from different monitoring organizations and analyzed by different laboratories will yield data of similar (comparable) quality. Therefore, the quality system will continue to strive for the development of data quality indicators and measurement quality objectives that will allow one to judge data quality and comparability and allow program managers to determine whether or not to require the use of a particular method (assuming this method meets the data quality needs). However, PBMS puts a premium on up-front planning and a commitment from monitoring organizations to adhere to implementing quality control requirements.

The data quality indicator **comparability** must be evaluated in light of a pollutant that is considered a **method-defined parameter**. The analytical result of a pollutant measurement, of a method-defined parameter, has a high dependence on the process used to make the measurement. Most analytical measurements are determinations of a definitive amount of a specific molecule or mixture of molecules. An example of this would be the concentration of carbon monoxide in ambient air. However, other

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[4] http://www.epa.gov/ttn/amtic/ncore/guidance.html

measurements are dependent on the process used to make the measurement. Method-defined parameters include measurements of physical parameters such as temperature and solar radiation which are dependent on the collection height and the design of the instrumentation used. Measurements of particulate mass, especially fine particulate, are also method-defined parameters because they are not "true" measures of particulate mass, being dependent on criteria such as: size cut-points which are geometrically defined; level of volatilization of particulates during sampling; and analytical methods that control the level of moisture associated with particulates at a concentration that may not represent actual conditions. (This should not be interpreted to mean that using a method-defined measurement of particulate is inferior. A "true" measurement of fine particulate in some environments can include a significant contribution from water, which is not a concern from a public/environmental health perspective).   When selecting methods or comparing data sets for method-defined parameter it is important to consider that there is no "correct" measurement only a "defined" method. However as mentioned above in the PBMS discussion, there are certain data quality acceptance limits for "defined" methods that can be used to accept alternative methods.

3.1 The DQO Process

The DQO process is used to facilitate the planning of EDOs. It asks the data user to focus their EDO efforts by specifying the use of the data (the decision), the decision criteria, and the probability they can accept making an incorrect decision based on the data. The DQO process:

- establishes a common language to be shared by decision makers, technical personnel, and statisticians in their discussion of program objectives and data quality;
- provides a mechanism to pare down a multitude of objectives into major critical questions;
- facilitates the development of clear statements of program objectives and constraints that will optimize data collection plans; and
- provides a logical structure within which an iterative process of guidance, design, and feedback may be accomplished efficiently.

The DQO process contains the following steps:

- **State the problem:** Define the problem that necessitates the study; identify the planning team, examine budget, schedule.

- **Identify the goal:** State how environmental data will be used in meeting objectives and solving the problem, identify study questions, define alternative outcomes.

- **Identify information inputs:** Identify data and information needed to answer study questions.

- **Define boundaries:** Specify the target population and characteristics of interest, define spatial and temporal limits, scale of inference.

- **Develop the analytical approach:** Define the parameter of interest, specify the type of inference, and develop the logic for drawing conclusions from findings.

- **Specify performance or acceptance criteria:**

    o *Decision making (hypothesis testing):* Specify probability limits for false rejection and false acceptance decision errors.

    o *Estimation approaches:* Develop performance criteria for new data being collected or acceptable criteria for existing data being considered for use.

- **Develop the plan for obtaining data:** Select the resource-effective sampling and analysis plan that meets the performance criteria.

The DQO Process is fully discussed in the document titled *Guidance on Systematic Planning using the Data Quality Objectives Process (EPA QA/G-4)*, and is available on the EPA's Quality System for Environmental Data and Technology website[5]. For an illustration of how the DQO process was applied to a particular ambient air monitoring problem, refer to the EPA document titled *Systematic Planning: A Case Study of Particulate Matter Ambient Air Monitoring*[6].

3.2 Ambient Air Quality DQOs

As indicated above, the first steps in the DQO process are to identify the problems that need to be resolved and the objectives to be met. As described in Section 2, the ambient air monitoring networks are designed to collect data to meet three basic objectives:

1. provide air pollution data to the general public in a timely manner;
2. support compliance with air quality standards and emission strategy development; and
3. support air pollution research.

These different objectives could potentially require different DQOs, making the development of DQOs complex. However, if one were to establish DQOs based upon the objective requiring the most stringent data quality requirements, one could assume that the other objectives could be met. Therefore, the DQOs have been initially established based upon ensuring that decision makers can make comparisons to the NAAQS within a specified degree of certainty. OAQPS has established formal DQOs for $PM_{2.5}$, Ozone, the NCore Precursor Gas Network, the $PM_{2.5}$ Speciation Trends Network (STN)[7], and the National Air Toxics Trends Network (NATTS)[8]. As the NAAQS for the other criteria pollutants come up for review, EPA will develop DQOs for these pollutants.

3.3 Measurement Quality Objectives

Once a DQO is established, the quality of the data must be evaluated and controlled to ensure that it is maintained within the established acceptance criteria. Measurement Quality Objectives (MQOs) are designed to evaluate and control various phases (e.g., sampling, transportation, preparation, analysis) of the measurement process to ensure that total measurement uncertainty is within the range prescribed by the DQOs. MQOs can be defined in terms of the following data quality indicators: precision, bias, representativeness, detection limit, completeness and comparability as described in Section 3.0.

MQOs can be established to evaluate overall measurement uncertainty, as well as for an individual phase of a measurement process. As an example, the precision DQO for $PM_{2.5}$ is 10% and it is based on 3 years of collocated precision data collected at a PQAO level. Since only 15% of the sites are collocated, the data can be used to control the quality from each site and since the results can be effected by field and laboratory processes one cannot pinpoint a specific phase of the measurement system when a precision result is higher than the 10% precision goal. Therefore individual precision values greater than 10% may be tolerated as long as the overall 3-year DQO is achieved. In contrast, the flow rate audit, which is specific to the appropriate functioning of the $PM_{2.5}$ sampler, has an MQO of $\pm$ 4% of the audit standard and $\pm$ 5% of the design value. This MQO must be met each time or the instrument is recalibrated. In summary, since uncertainty is usually additive, there is much less tolerance for uncertainty for individual

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[5] http://www.epa.gov/quality1/qa_docs.html
[6] http://www.epa.gov/quality1/qs-docs/casestudy2-final.pdf
[7] http://www.epa.gov/ttn/amtic/specguid.html
[8] http://www.epa.gov/ttn/amtic/airtoxqa.html

phases of a measurement system (e.g., flow rate) since each phase contributes to overall measurement. As monitoring organizations develop measurement specific MQOs they should think about being more stringent for individual phases of the measurement process since it will help to keep overall measurement uncertainty within acceptable levels.

For each of these indicators, acceptance criteria can be developed for various phases of the EDO. Various parts of 40 CFR Parts 50 and 58 have identified acceptance criteria for some of these indicators. In theory, if these MQOs are met, measurement uncertainty should be controlled to the levels required by the DQO. Table 3-1 is an example of an MQO table for ozone. MQO tables for the remaining criteria pollutants can be found in Appendix D. The ozone MQO table has been "re-developed" into what is known as a validation template. In June 1998, a workgroup of QA personnel from the monitoring organizations, EPA Regional Offices, and OAQPS was formed to develop a procedure that could be used by monitoring organizations for consistent use of MQOs and the validation of the criteria pollutants across the US. The workgroup developed three tables of criteria:

Critical Criteria- deemed critical to maintaining the integrity of a sample (or ambient air concentration value) or group of samples were placed on the first table. Observations that do not meet each and every criterion on the critical table should be invalidated unless there are compelling reason and justification for not doing so. Basically, the sample or group of samples for which one or more of these criteria are not met is invalid until proven otherwise.

Operational Criteria Table- important for maintaining and evaluating the quality of the data collection system. Violation of a criterion or a number of criteria may be cause for invalidation. The decision should consider other quality control information that may or may not indicate the data are acceptable for the parameter being controlled. Therefore, the sample or group of samples for which one or more of these criteria are not met is suspect unless other quality control information demonstrates otherwise. The reason for not meeting the criteria should be investigated, mitigated or justified.

Systematic Criteria Table- include those criteria which are important for the correct interpretation of the data but do not usually impact the validity of a sample or group of samples. For example, the data quality objectives are included in this table. If the data quality objectives are not met, this does not invalidate any of the samples but it may impact the error rate associated with the attainment/non-attainment decision.

More information about data validation and the use of the validation templates can be found in Section 17.

Table 3-1 Measurement Quality Objectives for Ozone Developed into a Validation Template

Requirement	Frequency	Acceptance Criteria
Critical Criteria		
One Point QC Check **Single analyzer**	1/ 2 weeks	$\leq$ 7% (percent difference)
Zero/span check	1/ 2 weeks	Zero drift # $\forall$ 3% of full scale Span drift # $\forall$ 7 %
Operational Criteria		
Shelter Temperature		
Temperature range	**Daily** (hourly values)	20 to 30E C. (Hourly ave) or per manufacturers specifications if designated to a wider temperature range
Temperature Control	Daily (hourly values)	# $\forall$ 2E C SD over 24 hours
Precision **(using 1-point QC checks)**	Calculated annually and as appropriate for design value estimates	90% CL CV $\leq$ 7%
Bias **(using 1-point QC checks)**	Calculated annually and as appropriate for design value estimates	95% CL $\leq$ $\pm$ 7%
Annual Performance Evaluation		
Single analyzer	Every site 1/year 25 % of sites quarterly	Percent difference at each audit level $\leq$ 15%
PQAO	annually	95% of audit percent differences fall within the one point QC check 95% probability intervals at PQAO level of aggregation
Federal Audits (NPAP)	1/year at selected sites 20% of sites audited	Mean absolute difference # 10%
State audits	1/year	State requirements
Calibration	Upon receipt/adjustment/repair and 1/6 months if manual zero/span performed biweekly 1/year if continuous zero/span performed daily	All points within $\forall$ 2 % of full scale of best-fit straight line
Zero Air		Concentrations below LDL
Gaseous Standards		NIST Traceable (e.g., EPA Protocol Gas)
Zero Air Check	1/year	Concentrations below LDL
Ozone Transfer standard		
Qualification and certification	Upon receipt of transfer standard	$\forall$4% or $\forall$4 ppb (whichever greater)
Recertification to local primary standard	Beginning and end of O3 season or 1/6 months whichever less	RSD of six slopes # 3.7% Std. Dev. of 6 intercepts 1.5 New slope = $\pm$ 0.05 of previous
Ozone local primary standard		
Certification/recertification to Standard Photometer	1/year	single point difference # $\forall$5 % (preferably $\forall$ 3%)
(if recertified via a transfer standard)	1/year	Regression slopes = 1.00 $\forall$ 0.03 and two intercepts are 0 $\forall$ 3 ppb
Detection		
Noise	NA	0.003 ppm
Systematic Criteria		
Standard Reporting Units	All data	ppm (final units in AQS)
Completeness (seasonal)	Daily	75% of hourly averages for the 8-hour period
Sample Residence Times		< 20 seconds
Sample Probe, Inlet, **Sampling train**		Pyrex Glass or Teflon
Siting		Un-obstructed probe inlet
EPA Standard Reference **Photometer Recertification**	1/year	Regression slope = 1.00 $\pm$ 0.01 and intercept < 3 ppb