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Developing Criteria for Equivalency Status for Continuous $PM_{2.5}$ Samplers

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Overview

- The $PM_{2.5}$ problem and a preview of PM_{Coarse}
- The basis of the solution
- The data to be collected & used
- The requirements / calculations
- $PM_{2.5}$ DQOs and the *DQO Companion* software
- Putting it all together
- Final Comments

The $PM_{2.5}$ Problem

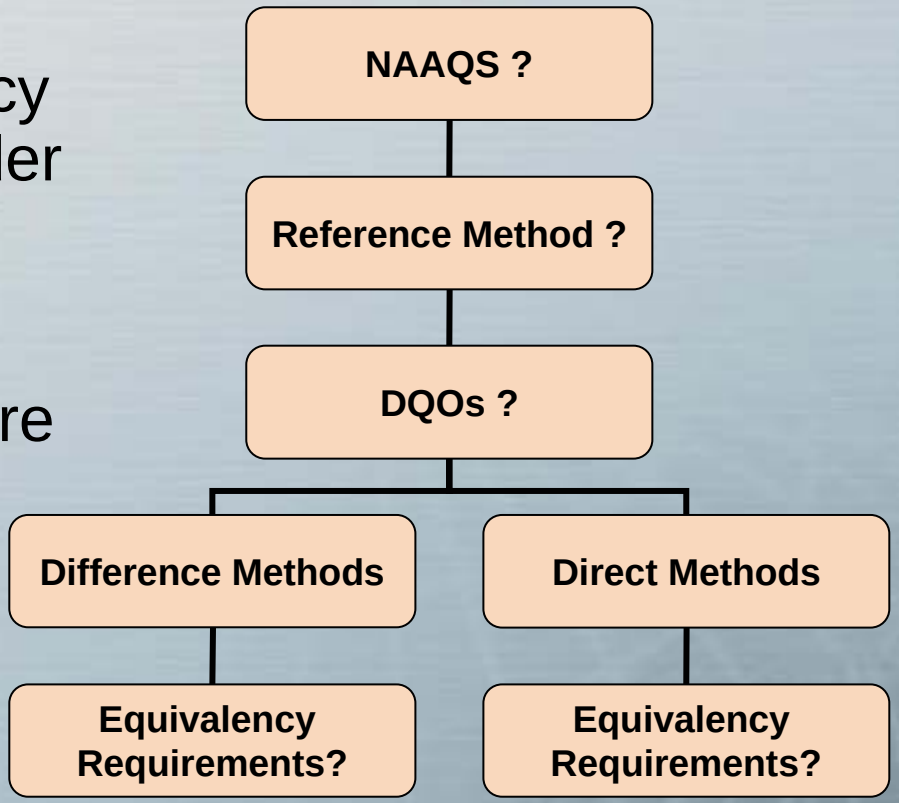
- How do we establish equivalency for continuous samplers or, more generally, Class III samplers in a way that is consistent with the DQOs?

Under 40 CFR Part 53, continuous samplers are defined as a Class III candidate method of sampling.

Class III equivalent methods include any candidate $PM_{2.5}$ methods that cannot qualify as either Class I or Class II. This class includes any filter-based integrated sampling method having other than a 24-hour $PM_{2.5}$ sample collection interval followed by moisture equilibrium and gravimetric mass. More importantly, Class III also includes filter-based continuous or semi-continuous methods, such as beta attenuation instruments, harmonic oscillating element instruments, and other complete in situ monitor types. Non-filter-based methods, such as nephelometry or other optical instruments, will also fall into the Class III category.

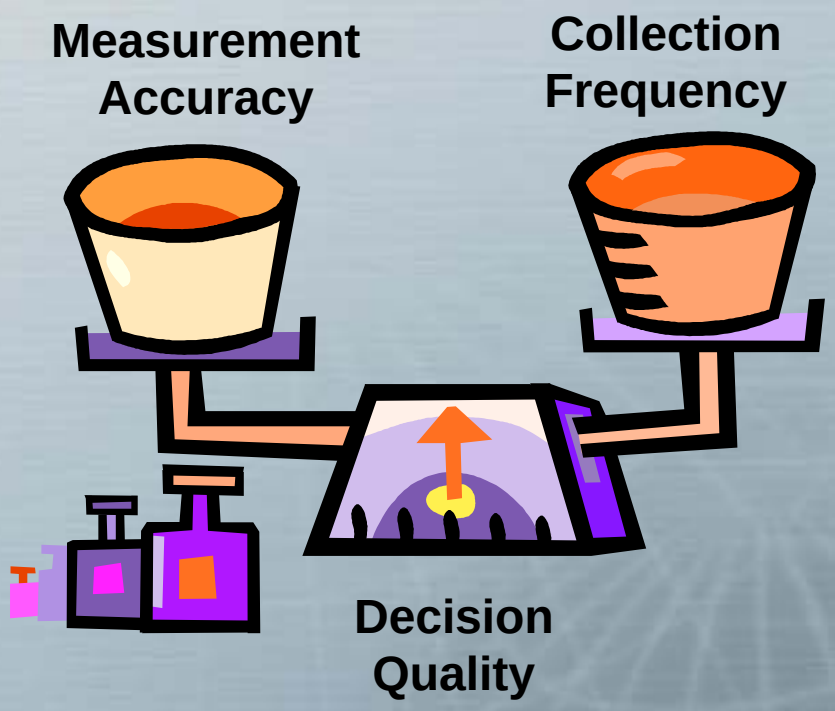
This is a Preview for PM_{Coarse}

- PM_{Coarse} DQOs and Equivalency requirements are currently under development.
- The problem for PM_{Coarse} is messier because there are more unknown aspects.



The Starting Point of the Solution

- The $PM_{2.5}$ DQOs are based on (among other assumptions) sampling every sixth day.
- The "continuous" methods produce data much more frequently than "every sixth day". This yields an opportunity for relaxed standards in the measurement accuracy while maintaining the same overall decision quality.
- The goal of this work was to develop an analytical connection between the DQOs and the change in sampling frequency with the usual methods for establishing equivalency.

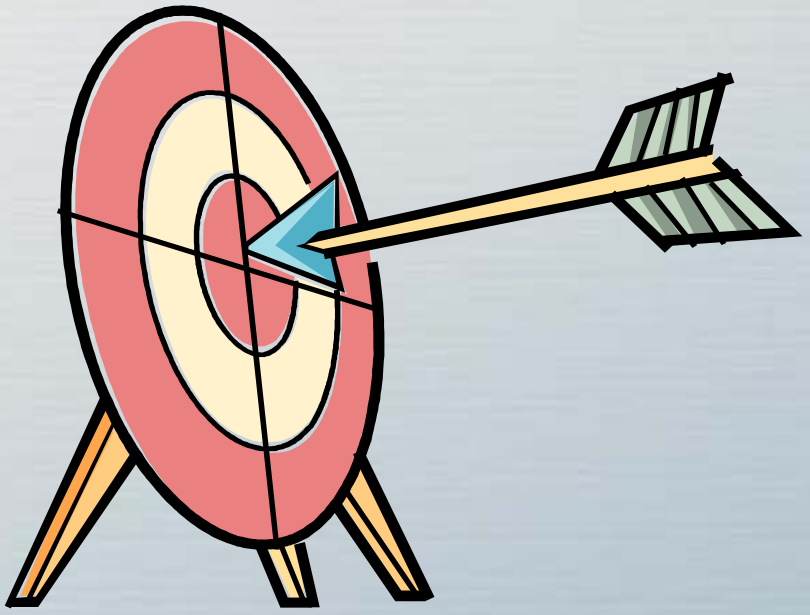


The Data

To determine the equivalency of a candidate continuous sampler relative to the FRM sampler, daily concentration data need to be obtained from $PM_{2.5}$ samples collected from collocated candidate and FRM samplers at multiple sites.

- **Three to five candidate samplers** will be collocated with **three FRM samplers**.
- Within a given season of the year, each sampler will be run daily for a **target of 30 days** (with at least one site having samples collected in multiple seasons).
- The required minimum sample collection period for each sampler is at least 22 hours.
- For data from a given day to be valid, valid data must be available for at least two FRM samplers and at least two candidate samplers.
- 75% completeness is required for each site and season. For a 30-day sampling period, this corresponds to a minimum of 23 days per season.
- The acceptable concentration range of sample data is 3 $\mu g/m^3$ to 200 $\mu g/m^3$.

From the Data We Want to Establish



- Precision
- Correlation
- Multiplicative bias
- Additive bias

Precision

The precision associated with the candidate sampler data is calculated as a root-mean-square:

$$Candidate\ \ precision = \sqrt{\frac{\sum_{i=1}^{D}\left(Cand.\ daily\ CV_i\right)^2}{D}}$$

where the summand is the daily coefficient of variation among the candidate samplers. The precision of the candidate sampler data must be **no greater than 15 percent** in order for the candidate sampler to qualify for equivalency classification**.**

This is the only “within day” statistic. Everything else is based on daily means.

Correlation — Calculation

Correlation in the daily means between the FRM and candidate samplers is calculated as follows:

$$r = \frac{D\sum_{i=1}^{D}\left(FRM\ daily\ mean_i \cdot Cand.\ daily\ mean_i\right) - \left(\sum_{i=1}^{D} FRM\ daily\ mean_i\right)\cdot\left(\sum_{i=1}^{D} Cand.\ daily\ mean_i\right)}{D^2 \cdot Cand.\ RMS \cdot FRM\ RMS}$$

where "*Cand. RMS*" and "*FRM RMS*" are the root-mean-square deviations from the overall means of the daily means for the candidate and FRM samplers.

This is the standard Correlation Coefficient between the daily means of the FRM samplers and the daily means of the candidate samplers.

Correlation — Requirement

The Correlation coefficient needs to be above:

$$Correlation\ lower\,bound(CCV) = \begin{cases} 0.93 & if \quad CCV < 0.3 \\ 0.87 + 0.2 \cdot CCV & if \quad 0.3 \le CCV < 0.4 \\ 0.95 & if \quad 0.4 \le CCV \end{cases}$$

where CCV is the coefficient of variation of the daily means of the FRM samplers (the population CV of the FRM daily means).

[We will come back to where this formula came from.]

Multiplicative Bias

The multiplicative bias is the slope of the ordinary least-squares line between the daily means of the candidate and FRM samplers:

$$b = r \cdot \frac{Cand.\ RMS}{FRM\ \ RMS}$$

The multiplicative bias associated with the candidate sampler **must fall between 0.90 and 1.10** in order for the candidate sampler to qualify for equivalency classification.

(Subtract 1 and you get the usual +/- 10%.)

Additive Bias — Calculation

The additive bias is the intercept of the ordinary least-squares line between the daily means of the candidate and FRM samplers.

$$a = \left(\frac{1}{D} \cdot \sum_{i=1}^{D} Cand.\,daily\ mean_i \right) - b \cdot Overall\ \ FRM\ \ mean$$

where b is the slope estimate (multiplicative bias) and the overall mean is calculated from the FRM samplers.

Additive Bias — Requirement

The additive bias associated with the candidate sampler **must fall between $a_1(b)$ and $a_2(b)$** in order to qualify for equivalency classification. These lower and upper bounds, which are linear functions of the multiplicative bias, are as follows:

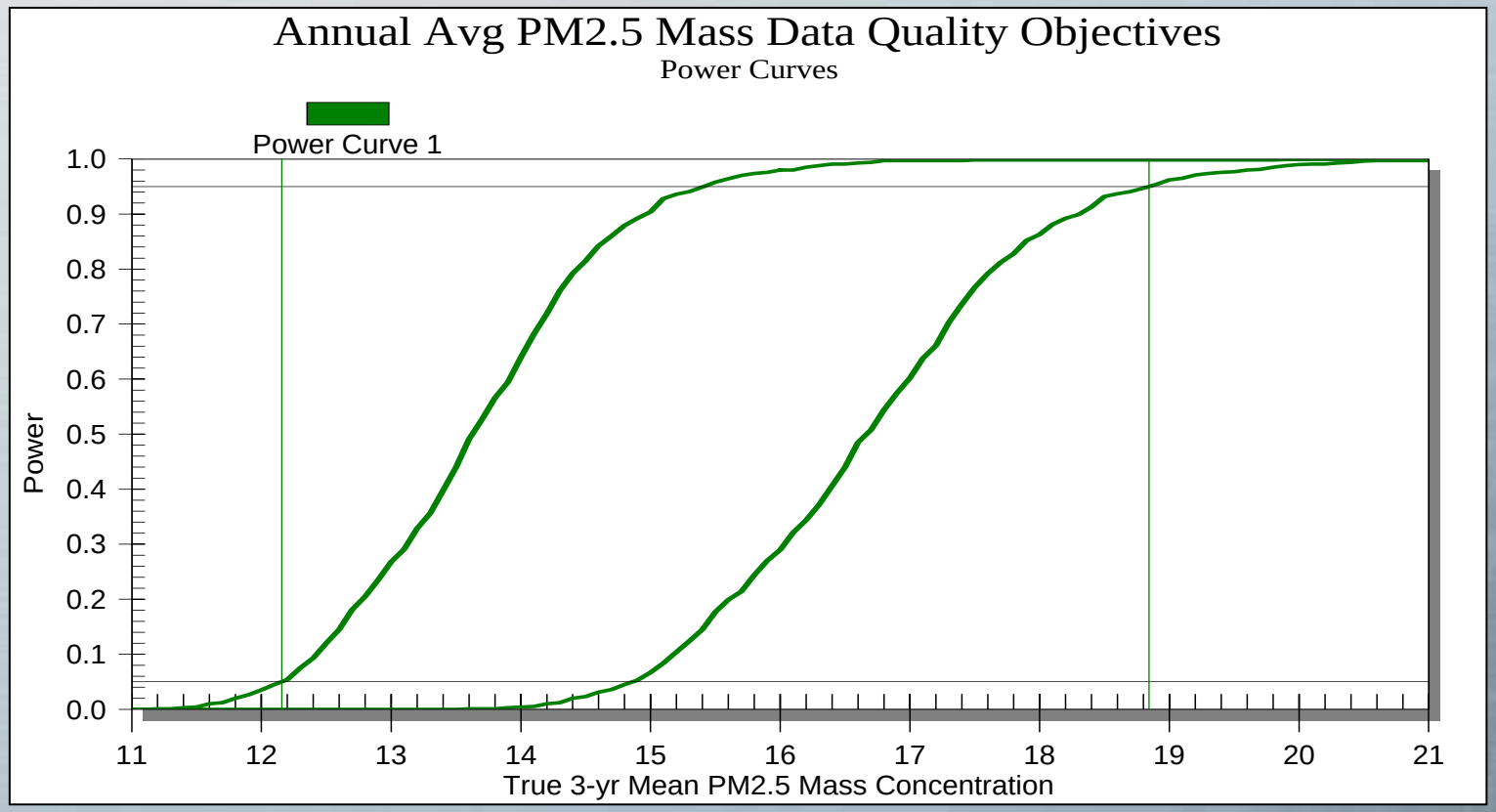
$$a_1(b) = 15.05 - 0.92(18.8)b = 15.05 - 17.31b$$

$$a_2(b) = 15.05 - 1.08(12.2)b = 15.05 - 13.20b$$

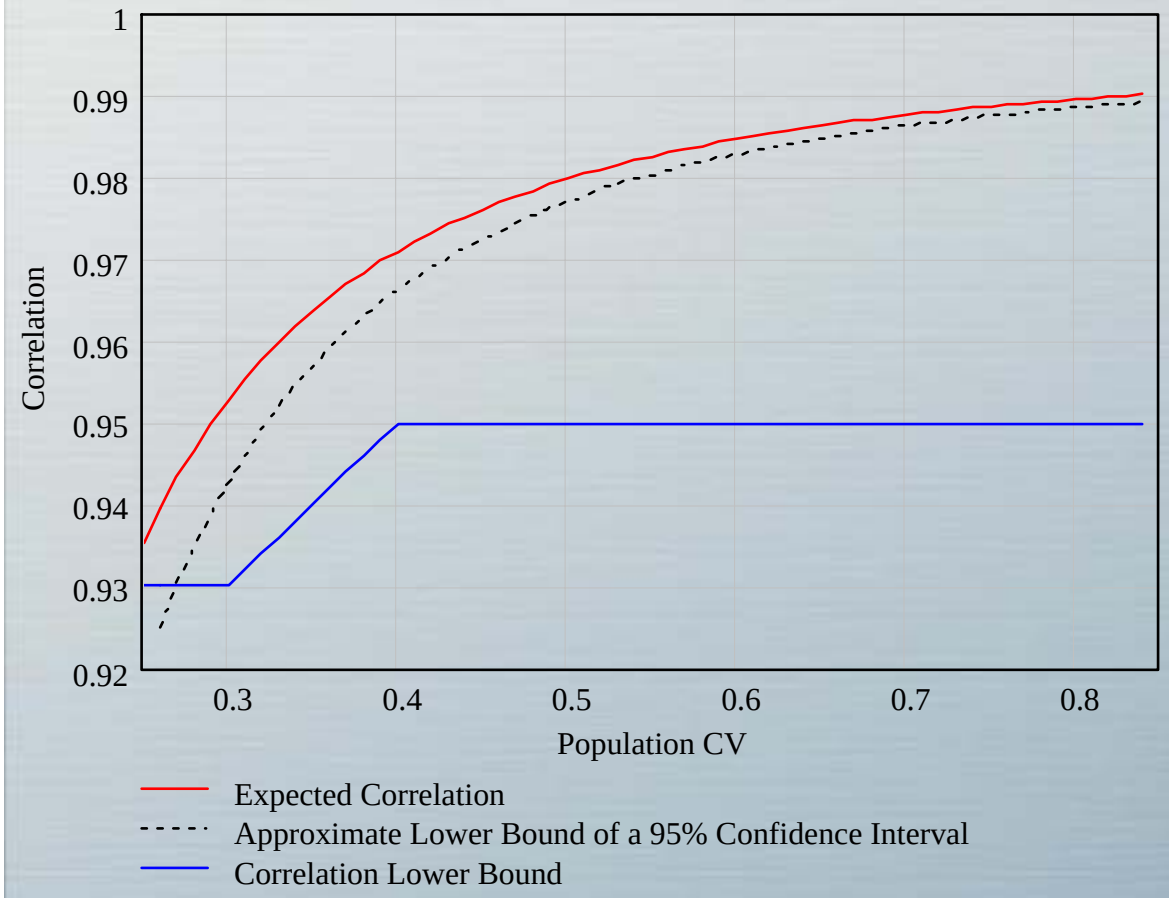
These lines are based on the DQOs and allow for additional additive bias that can be absorbed because the sampling frequency for these methods is daily.

$PM_{2.5}$ DQOs and the *DQO Companion* software

The $PM_{2.5}$ DQOs are based on a statistical simulation of every sixth day sampling that yields a gray zone of 12.2 to 18.8 μg/m³. The parameters that go into the simulation can be investigated with the *DQO Companion* software developed by Battelle for EPA. These include: completeness, sampling frequency, natural variation, and measurement errors.



Expected Correlation and the Lower Limit



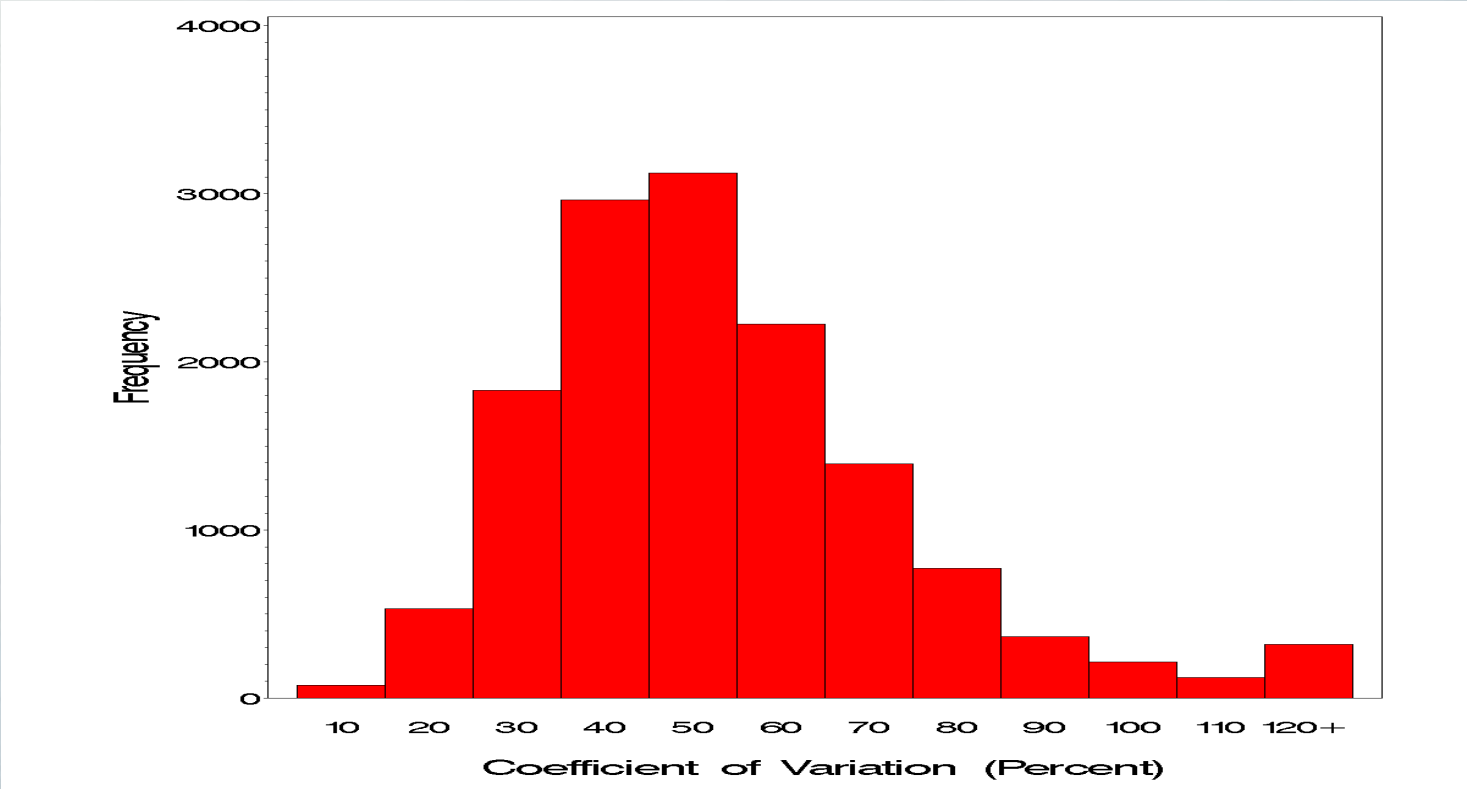
It turns out that the expected correlation depends on the population CV.

In most regression problems this is bad news.

For $PM_{2.5}$, the population CV varies from site-to-site, but is fairly constant through time.

This means that test sites should be chosen where the CV has been historically large.

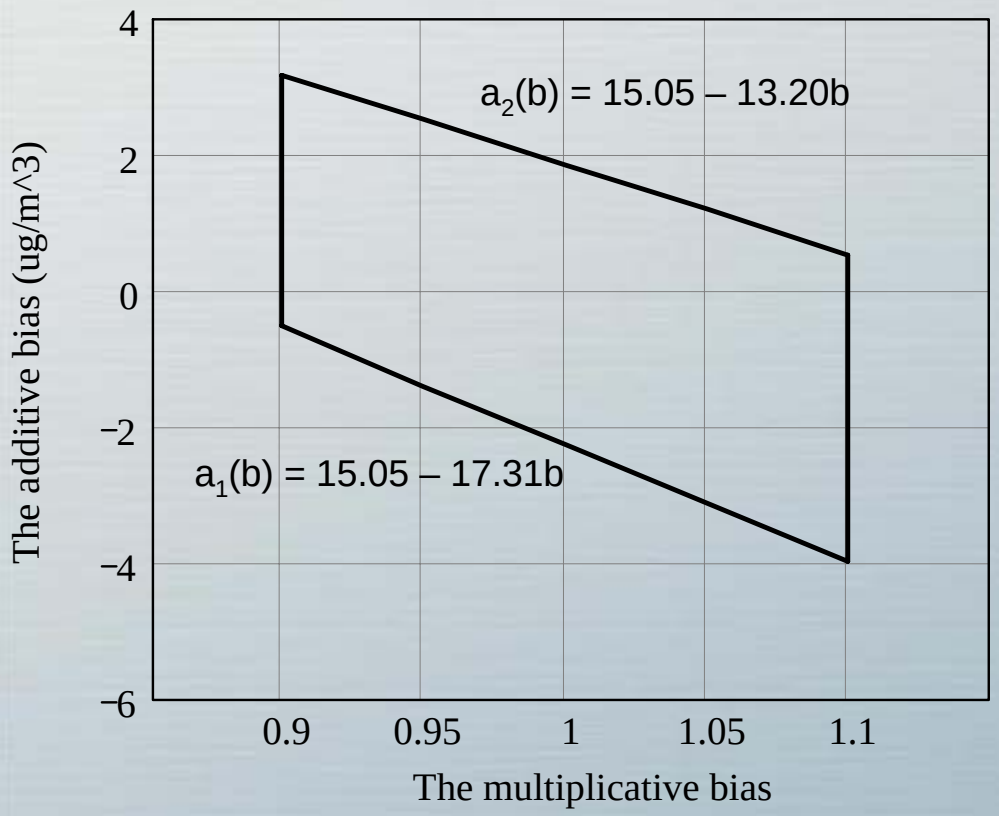
Typical Population CV's



Monthly population CV's calculated from 2003 data.

** The CV dependence is not a problem. **

The Bias Terms



Once linear fit has been established, the usual linear regression can be used to find the multiplicative and additive components of the bias.

- Both components are seen in real data from semi-continuous instruments.
- The multiplicative bias is held at ±10%.
- The limits on the additive portion depend on the multiplicative portion.

The Origin of the Additive Bias Limits (1)

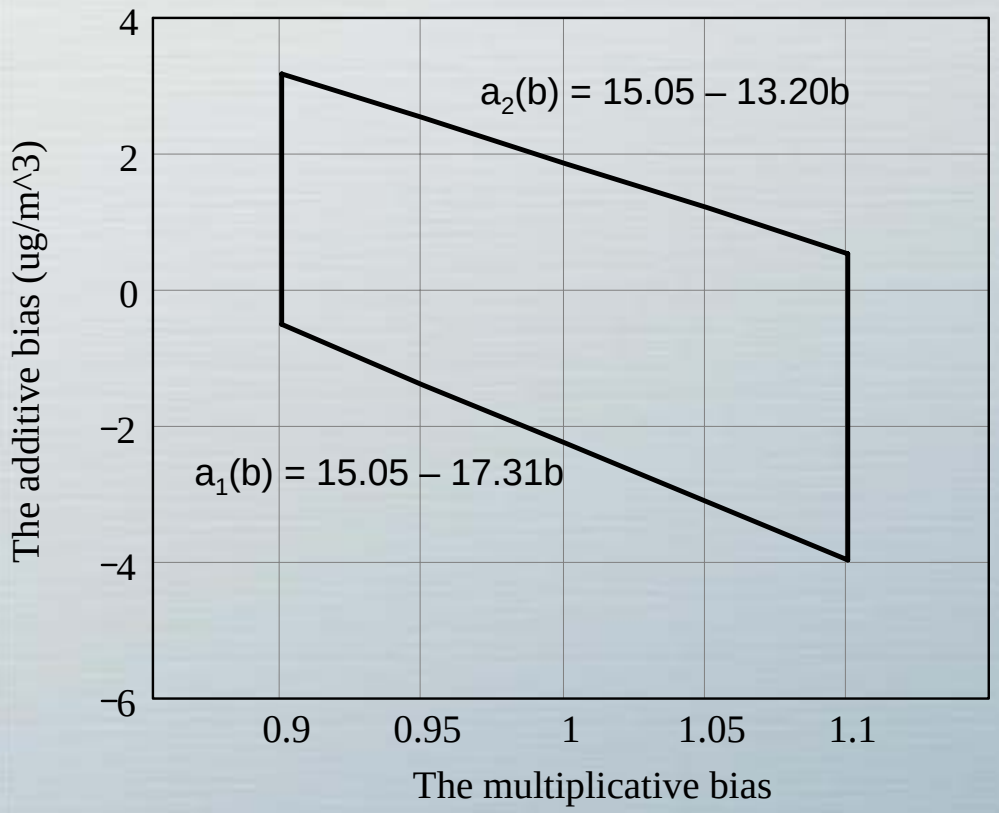
- The gray zone limits come from simulations with random measurement error and statistical sampling error (the error associated with data incompleteness) with the biases applied at the end.
- Running the *DQO Companion* software with every 3rd day sampling yields a gray zone of about 12.64 to 18.16.
- We want to find the 5th and 95th percentiles of the simulations.

$$15.05 - 18.16(0.9)x = 0 \quad \text{or} \quad x = 0.92$$

$$15.05 - 12.64(1.1)y = 0 \quad \text{or} \quad y = 1.08$$

(Only 5% of the time, the simulations have 3-year means that are less than 92% of the truth.)

The Origin of the Additive Bias Limits (2)



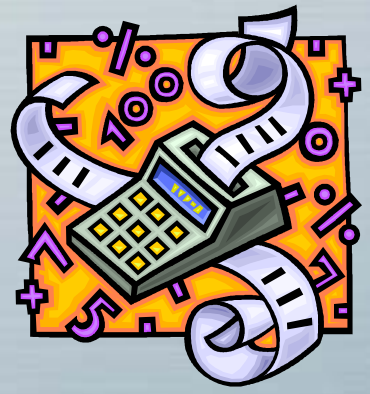
Now we map those simulations back to a combination of additive and multiplicative biases that would yield the original 12.2 to 18.8 gray zone.

$$a_1(b) = 15.05 – 0.92(18.8)b$$
$$= 15.05 – 17.31b$$

$$a_2(b) = 15.05 – 1.08(12.2)b$$
$$= 15.05 – 13.20b$$

Note that the additive bias and the multiplicative biases can have different signs and compensate so long as the overall effect yields a gray zone within12.2 to 18.8 and the multiplicative bias is at most 10%.

Final Comments



- The calculations for establishing equivalency include a precision calculation and the usual calculations based on linear regression against the standard: correlation, intercept, and slope.
- The requirements are derived from the $PM_{2.5}$ DQO simulation model.
- Manufacturers can help themselves meet the correlation requirement by choosing sites with a high population CV.
  - Such a choice will also increase the precision of the estimates for additive and multiplicative bias.
  - The CV tends to be fairly constant through time for a fixed site and there are ample historical data available for making selections.