Guideline on Air Quality Models
March 19-21, 2013
Sheraton Raleigh Hotel, Raleigh, N.C

Pounding Nails with Shoes to Decide Which Shoes to Buy

By
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Retired NOAA (2004)
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Venkatram, A. (1979): The expected deviation of observed concentrations from predicted ensemble means. Atmos. Environ. (11):1547-1549. "…we expect the 1-h averaged concentration to deviate from the ensemble mean by more than 100%. …"

Fox, D.G. (1984): Uncertainty in air quality modeling. Bull. Amer. Meteoro. Soc. (65):27-36. "…In studies of turbulence, it is convenient to introduce the notion of an ensemble, namely a number of repeats of the same 'experiment,' holding external conditions (boundary and initial conditions) fixed…."

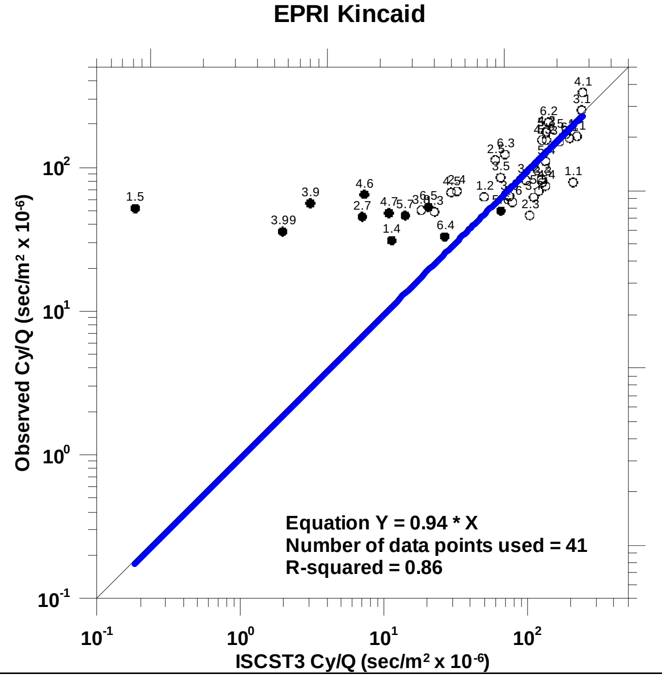
Weil, J.C., R.I. Sykes, and A. Venkatram (1992): Evaluating air-quality models: review and outlook. Journal of Applied Meteoro. ((31):1121-1145. "…Air-quality models predict the mean concentration for a given set of conditions (i.e., an ensemble), whereas observations are individual realizations drawn from the ensemble."

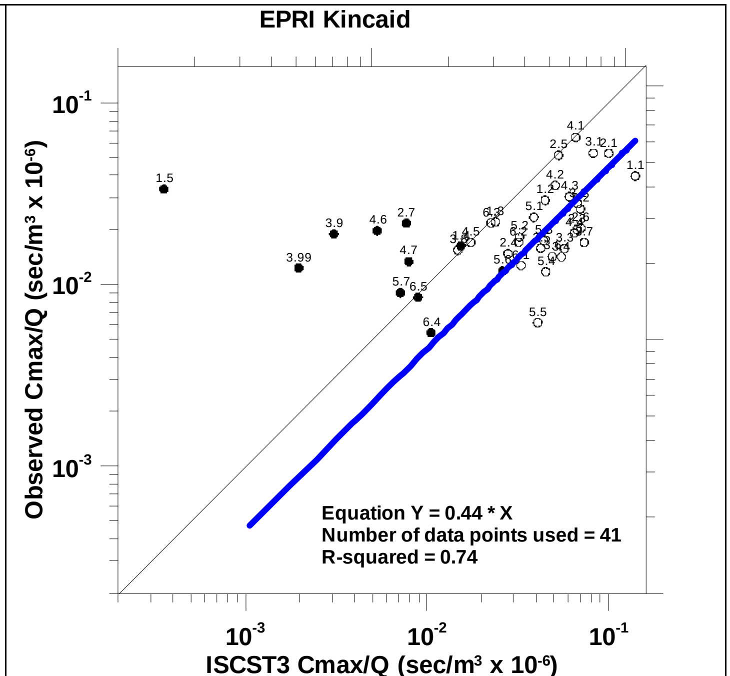
If arc-maxima differ so greatly from the ensemble maxima, why are we comparing arc-maxima with dispersion model ensemble-average maxima to assess model performance?

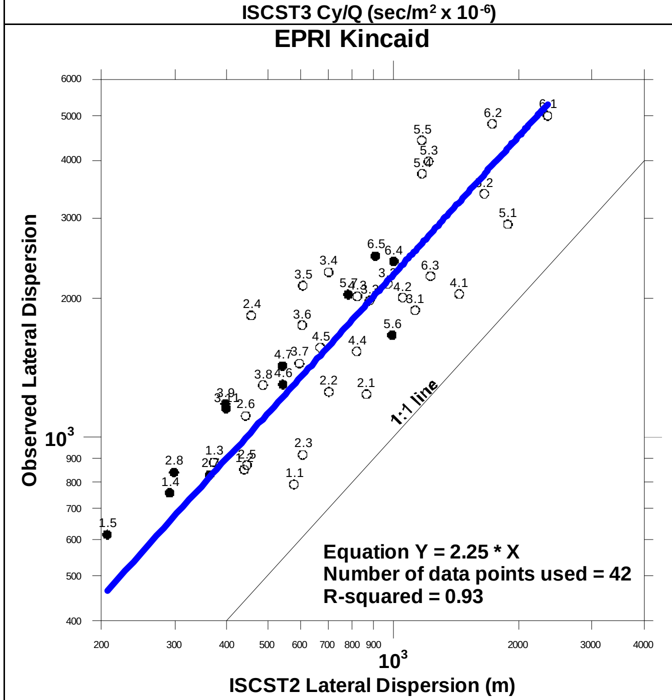
MY VENT:
You can use a shoe to pound nails into a board. You can even decide which shoes to buy based on their ability to pound nails into a board. But shoes were never made to pound nails, and their ability to pound nails into a board makes for terrible selection criteria as to which shoes to buy!

Dispersion models were never constructed to estimate short-term maxima. You can misconstrue what dispersion models do and say they estimate individual realization maxima; you can even try to assess dispersion model performance by comparing model estimates with individual realization maxima.

It makes no sense to select shoes on their ability to pound nails, nor does it make sense to assess dispersion model performance through comparisons of modeling results with short-term arc-maxima.





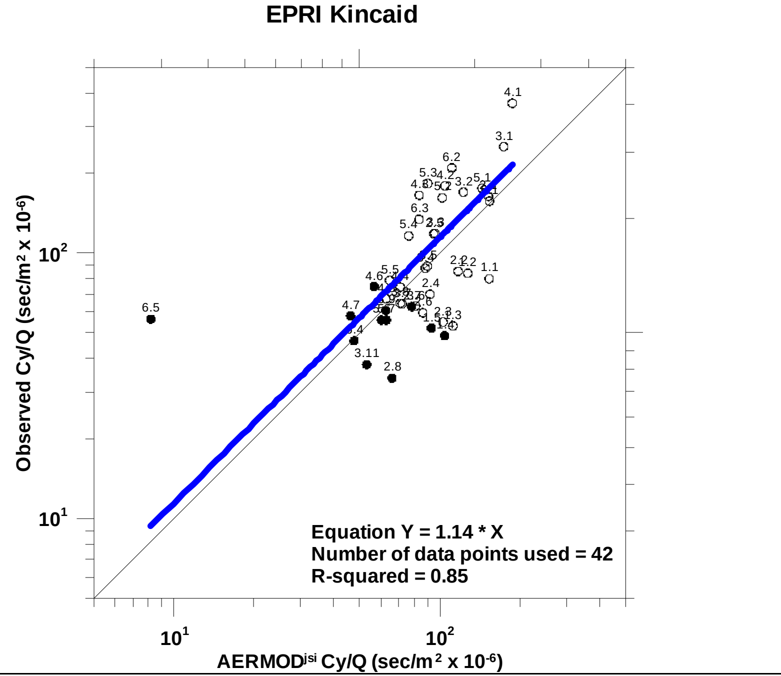


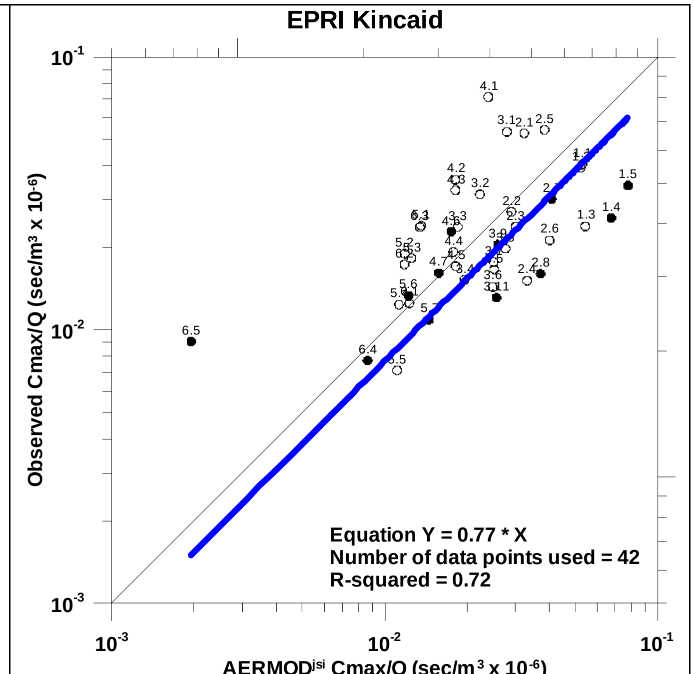
$$C_{\max}(x,0,0,H) = \frac{C_y}{\sqrt{2\pi}\sigma_y}$$

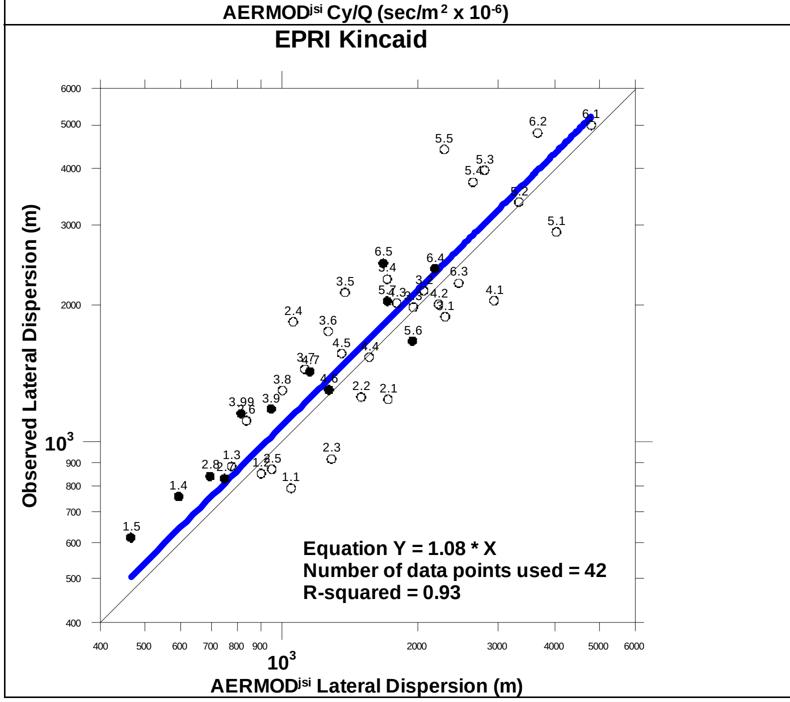
Symbol Labels:
First number refers to arc. I used six Kincaid arcs: 1=3, 2=5, 3=7, 4=10, 5=15, and 6=20km.

I group the data into 10-value geometric averages, going from most unstable to stable. A symbol label of 1.1 = 3km most unstable group; 3.9 = 7km nearly stable group. Open symbols = unstable; solid symbols = most neutral/stable.

ISCST3 (v 02035)







$$C_{\max}(x,0,0,H) = \frac{C_y}{\sqrt{2\pi}\sigma_y}$$

Notice how the over-estimation of Cy is amplified by the under-estimation of Sy, resulting in large over-estimates of Cmax.

AERMOD (v 12345)

Summary of lessons learned (I hope):

1. All air-quality models (ISCST3, AERMOD, ADMS, CMAQ, CAMx, etc.) provide estimates of the ensemble average concentration. Direct comparisons of short-term (1-hour or less) observations with modeling results is highly questionable. There are large stochastic fluctuations affecting short-term concentration values, which prohibit meaningful comparison between modeled ensemble averages with short-term concentration values.

2. For dispersion models like AERMOD, I am recommending comparisons of group geometric mean values of observed and estimated Cy and Sy values. Once you understand what is happening with Cy and Sy, you can look at Cmax. <u>We place too much emphasis on the importance of Cmax in our model evaluations; Cmax is dependent upon Cy and Sy (not the other way around).</u>

a. I suggest using log scales on both the x- and y-axis so we can see what is happening with the small values, as well as the large values.

b. I suggest using an ordinary least-square fit forcing the intercept to be zero, to provide a quick overall average assessment of bias, but as you will see, it is not always useful.

c. I suggest placing the modeled values on the x-axis since ordinary least-square fits assume the uncertainty to be in the y-axis values, which in our case are the observations, which we know should have larger variances than the deterministic model values due to unresolved stochastic processes.

c. I suggest you use labels on the plot symbols. 1, 2, 3, …5 to denote which arc: 1 = 50m and 5 = 800m. The decimals denote stability, so 1.1 is the 50m arc and the most unstable group, and 4.6 is the 800m arc and the most stable group. To further help, I have used solid black symbols for the most stable two groups on each arc.

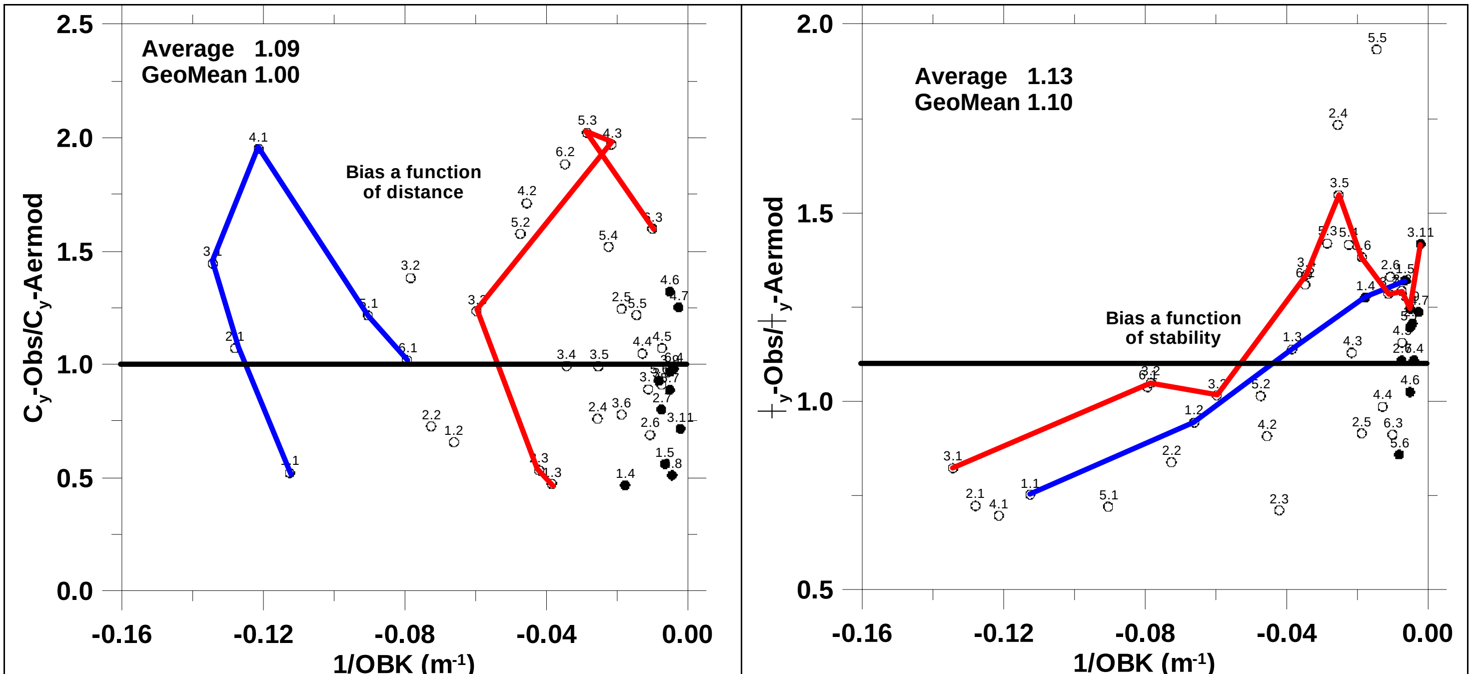
The use of geometric means insures a science basis in the relationship between Cy, Sy and Cmax. You should not deviate on this. The use of log scales on x- and y-axis; least-square fits forcing the intercept to be zero, and labeling the symbols are what I call ‘good-practices’ developed from experience; trial and error. They are worth using initially until we devise something better.

3. It is my contention that there is no science or statistical basis for assessing model performance using observed short-term arc-maxima values. You can pound nails with shoes to decide which shoes to buy and you can attempt to assess dispersion model performance through a comparison of model estimates with observed arc-maxima values.

Neither of these activities makes good sense!

Selecting only the short-term arc-maxima from intensive field data sets for evaluation of dispersion model performance makes very poor use of available data and does a poor job of revealing the underlying model biases.

We have not pinpointed what has to be done to AERMOD (v12345) to reduce the biases seen in C_y and σ_y, but we have clues.



The above plots were constructed using the 10-value geometric group averages for the observed and AERMOD crosswind integrated concentration values (C_y) and lateral dispersion values (σ_y). In defining the 10-value groups, I made no effort to force the stability-ranges to be the same for each downwind distance.

The overall bias in C_y is about 1.0 and in σ_y is about 1.10, but the bias in C_y varies by distance and the bias in σ_y varies by stability. This shows that to understand the centerline concentration values (C_{max}) we need to separately understand what is happening with C_y and σ_y.