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**Analysis Steps Conducted for Presentation Entitled
Pounding Nails With Shoes To Decide Which Shoes To Buy**

By

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This discussion provides some of the details of the analyses conducted to develop the invited luncheon talk for the AW&MA Guideline on Air Quality Models March 19-21, 2013 at the Sheraton Raleigh Hotel, Raleigh, N.C.

Crosswind integrated concentration (C_y)

Laateral dispersion (S_y)

Gaussian fit centerline maximum concentration (C_{max})

Appendix A: Analysis Steps

1. Compute C_y , S_y and C_{max} from observations
 - a. While listing out the computed C_y , S_y and C_{max} values, I converted the Project Prairie Grass concentrations from milligrams/ m^3 to micrograms/ m^3 .
 - b While listing out the computed C_y , S_y and C_{max} values, I converted the Kincaid concentrations from PPB to micrograms/ m^3 , and I listed to a separate file the Kincaid stack parameters in AERMOD's format of hourly emission rates. Note, ISCST3 and AERMOD share the same hourly emission input file format.
 - c. I wrote a program to read my master file of quality codes and from this I determined that there were six arcs where I likely had sufficient data to form and use group averages sorted by stability, namely: 3, 5, 7, 10, 15, and 20km.
2. Define Dates –
 - a. Since I am using all 68 experiments initially, I just listed to a side file the 68 dates and times.
 - b. For EPRI Kinciad, I only need ISCST3 and AERMOD modeling results for those hours when I have valid observed values for C_y , S_y and C_{max} . I created a program to read the Kincaid file of C_y , S_y and C_{max} results computed in Step 1, which then listed out the hours for which I need modeling results.
3. AERMET meteorology –Note I have fixed the wind direction to be coming from the west, as this simplifies Steps 5 and 6. More discussion in Appendix B.
4. CutMet - Using the listing of dates defined in Step 2, I extracted from the AERMET surf and prof data files, those hours for which I needed modeling results. As I did this, I created the meteorology input file for ISCST3, which required me to convert the Monin-Obukhov length to a Pasquill stability category. More discussion in Appendix B.

5. Define Receptors – I created a program where you tell it the distances downwind in meters; the starting azimuth, the spacing between receptors in degrees, and the number of receptors on each arc. The program creates the receptors, one arc at a time, and lists the coordinates in a format that can be used directly in ISCST3 and AERMOD. For Project Prairie Grass, I created 120 receptors with 1-degree separation on 5 arcs (50, 100, 200, 400, and 800m). For Kincaid, I created 300 receptors with 0.5-degree separation on 6 arcs (3, 5, 7, 10, 15, 20-km). I did not use actual ground elevations for the receptors, i.e. I assumed a flat world.

6. Model runs – Since I am dividing all concentration by the emission rate, I set the emission rate to be 1000 g/s, to insure that I would have nonzero concentrations even out to 50km. The concentration listed in the plot files of AERMOD and ISCST3 are in micrograms/m³. More discussion in Appendix C.

7. Compute Cy, Sy and Cmax from modeling results – The format of the plot files created by ISCST3 and AERMOD are slightly different, but the first line of their respective files provides the model name and version number, so I can use one program to process the modeling results from both models. I know from Step 5 how many receptors NUM are along each arc, so I read NUM concentrations in: compute Cy, Sy and Cmax, list out the results, and go to the next NUM of receptors to process. More discussion in Appendix D.

8. Combine Results –

a. For Project Prairie Grass, I computed observed values of Cy, Sy and Cmax for all 5 arcs and all 68 experiments, and I computed Cy, Sy and Cmax for all 5 arcs and all 68 experiments. I combined the observation results and modeling results in an Excel spreadsheet. I pulled the AERMET surf file into an Excel spreadsheet, and extracted AERMET's Monin-Obukhov length, which I then copied and pasted into my file of combined results for Project Prairie Grass.

b. For Kincaid, I computed Cy, Sy and Cmax from the observations results for all arcs having a Quality Code of 3, regardless of how far downwind the arc was. Since I have modeling results for 6 arcs, but may or may not have results for any or only some of the arcs, I wrote a program to combine the observed, ISCST3 and AERMOD Cy, Sy and Cmax values into one file. While doing this, I listed out AERMET's Monin-Obukhov length for each combined listing. Once I had the combined listing, I pulled the results into an Excel spreadsheet.

9. Form Groups – I use Golden Software Grapher, which allows me to create all my plots using data stored in Excel spreadsheets.

a. I started with Project Prairie Grass, doing a combined sort first on distance and then on 1/OBK. I then inserted columns where needed and created 10-value averages of observed and modeled Cy, Sy and Cmax. I had 65 values with which to work, but only used the first 60, which left out the 5 most stable values.

b. I then sorted the Kincaid combined data, and computed 10-value averages, leaving out a few of the most stable values, as in processing the Project Prairie Grass data into group averages.

c. While looking at the results, I decided to add the least square fits forced to have a zero intercept. I could not see what was happening for the low values, so I changed all the plots from linear to log axes. Then I added the labels to the symbols, to see whether I could see any trends. It was after all of the above, that I saw that the arithmetic 10-value averages were not obeying the relationship between C_{max} , C_y and S_y . I tried geometric 10-value averages, and I found that the relationship between C_{max} , C_y and S_y was preserved. This is a brief summary of the redoes I went through to come to a final set of plots and analyses.

Appendix B: Meteorology Processing

a. Source for data - Integrated Surface Database (ISD), Hourly, Global

<http://www.ncdc.noaa.gov/most-popular-data#dsi-3505>

b. Reformatting of data – AERMET can not read the ISD data as delivered, so I wrote a program that fakes it into the CD144 format, which AERMET can read. I set the wind direction to 270 degrees, to simplify defining the receptor rings for use in AERMOD and ISCST3. (**CDO2CD144.exe**)

c. I noticed that I had hours with zero wind speeds here and there in the data that I had created in CD144 format. My purpose is to demonstrate a methodology for evaluation of plume dispersion models, not make the definitive assessment. Hence, I use linear interpolation and filled in calm wind hours. (**FillCD144.exe**)

d. I have to run consecutive hours through AERMET to generate the input meteorology for AERMOD, because AERMET using 3-hr averaging to define the stable mixing height. However once the meteorology is developed, I can omit all hours except those for which I need AERMOD results. I created a program that reads a user define file of dates (and hours) for which I want AERMOD results, and the program: 1) list to a file the needed surface and profile data for each needed hour, and 2) creates the ISCST3 input meteorology data. AERMET had all the needed meteorology except for a Pasquill stability category, which I could estimate using the AERMET Obukhov length and the site roughness length. (**MyCutAERISC.exe**)

Note: I created a program to list the needed Dates and Times for EPRI Kincaid (see Appendix D b iv).

Appendix C: Dispersion Modeling Processing

a. AERMOD Plume Meander – One of the ‘tricks’ I am using to perform my analyses is to compute the modeled crosswind integrated concentration, C_y , and the lateral dispersion, S_y , using concentrations along receptor rings. In default mode, AERMOD’s plume meander will compute nonzero concentrations essentially in all directions, which does not realistically replicate what we see during the intensive field experiments. So I used the non-default model option LOWWIND1 to turn off AERMOD’s plume meander. All my AERMOD input files contained the following statement:

MODELOPT BETA CONC NOCHKD FLAT LOWWIND1

b. Receptor Field – I did not consider the ground elevation to be of any significance for the two intensive field experiments that I used in my analyses. However, I needed an easy way to generate receptors along rings at specified distances and separation. AERMOD and ISCST3 use the same flagpole receptor format, so I create a program to list out the needed receptors in the proper format, which I then cut and pasted into the input files for AERMOD and ISCST3. (**MakeReceptors.exe**)

c. Both AERMOD and ISCST3 will list out the concentrations generated at each file in a ‘plot’ format. All my input files contained a statement similar to the following:

POSTFILE 1 ALL PLOT KINSF6-1981.PST

The only thing that changed was the filename. If you have 120 receptors, then for each hour, the ISCST3 and AERMOD list out 120 concentrations. I created a program that reads the plot files, and computes the C_y , S_y and C_{max} values for each arc from the modeling results. (**AZRingAnalysis.exe**)

Appendix D: Observations Processing

Observations – The format of the Project Prairie Grass and EPRI Kincaid observations are slightly different, with different data included in the headers for each arc. I used the same subroutines to compute C_y , S_y and C_{max} , but created separate programs for each field data. The input files have the actual emission rates, so when listing out C_y and C_{max} , I divided these values by the emission rates.

a. Project Prairie Grass. The Project Prairie Grass results are recorded in milligrams per meter cubed, which I converted to micrograms per meter cubed (for comparison to the modeling results). (**PGRAnalysis.exe**)

b. EPRI Kincaid.

(i) The EPRI Kincaid results are recorded in PPB, which I converted to micrograms per meter cubed (for comparison to the modeling results). The conversion is in the header record for each hour and arc.

(ii). There is plume rise for the EPRI Kincaid experiments, so while listing out the observed values of C_y , S_y and C_{max} , I created an hourly emissions file in AERMOD's format (which is the same for ISCST3).

(iii) I used only those arcs that had a quality code of 3 (which means the observed maximum was in the middle third of the observed concentrations along the arc, the observed maximum looked to be in accord with concentrations seen along arcs in front and behind, and there were at least 5 nonzero concentrations along the arc).

(**KINAnalysis.exe**)

(iv) Kincaid Modeling Dates. Once I computed the observed values for C_y , S_y and C_{max} , I created a program that used the file created KINAnalysis to create a listing of the dates and hours for which I need modeling results for the Kincaid experiments. This listing of dates and times was used by MyCutAERISC (see Appendix B d 2).

(**KINDefineDates.exe**)

Appendix E: Final Processing

a. Project Prairie Grass. Once the AERMOD and ISCST3 modeling results were processed by AZRingAnalysis, I combined these results with those generated by PGRAnalysis in Excel, where I formed 10-group averages for plotting and analysis.

b. EPRI Kincaid.

(i) Once the AERMOD and ISCST3 modeling results were processed by AZRingAnalysis, I combined these results with those generated by KINAnalysis using a program I created. (**KINCombineAll.exe**)

(ii) I converted the combined file into an Excel file, where I formed 10-group averages for plotting and analysis.