**Evaluating the Performance of the WSAQS Photochemical Grid Model Platform**

**Statistical and Graphical Displays Checklist**

**ASSESSMENT OF BOUNDARY CONDITIONS**

Recommended graphical displays:

1. Spatial, timeseries, and vertical displays that evaluate ozone, ozone precursors, PM2.5, and speciated PM2.5., stratospheric intrusions, fires, dust, methane.
2. The analysis would focus on the boundaries and individual rural or remote sites.
3. These types of plots will aid in identifying days on which the model has high background levels.
4. The results will also be useful for comparison with subsequent model simulations with anthropogenic emissions to assess the contribution of anthropogenic emissions to O3 and PM2.5.

**ASSESSMENT OF EMISSIONS INVENTORY AND MODELING RESULT**S

Recommended quality assurance activities:

1. Check inventory data codes to ensure they are valid codes.
2. Compare post-SMOKE annual totals with Emissions Modeling Framework (EMF) inventory totals; usual tolerance is 1.0% or less
3. Ensure sources are identified properly, are not double-counted across point and nonpoint, and do not have missing pollutant emission rates, missing temporal allocations or missing spatial components.
4. Rank emissions and calculate percent differences with previous emissions estimates
5. Compare previous emissions, new (or proposed) emissions, region-by-region emissions, and the computed difference or percent difference side-by-side.
6. This analysis should be done one pollutant at a time for the following: analyzing NOx, VOCs, NH3, CH4,[[1]](#footnote-2) SO2, PM2.5, PM10, and PMC, and all source categories.

Recommended graphical displays:

1. Map emissions values for individual SCCs, groups of SCCs, county level emissions, and emissions differences among inventories
2. Spatial plots with pie charts for each county of the various source category contributions by pollutant and region.
3. Bar plots of source category contributions by county by pollutant.
4. Tabulate the significant sources (SCC) contributing to each source category by pollutant and region.
5. Pie Chart of Spatial, Temporal, and Chemical Allocations by source category by pollutant.
6. Bar, spatial, and pie plots of VOC Reactivity Analysis (RTOG/TOG)[[2]](#footnote-3) for various source category contributions by region.
7. Plots and Tables of spatial and temporal allocations and chemical speciation assignments.
8. Comparison to previous emissions modeling efforts to verify expected emissions changes by source category(s) and geographic area(s) of interest.
   1. Bar plots of annual emissions contributions of source categories by pollutant and region.
   2. Trends tables between years for various sectors and pollutants by region.
   3. Bar plots of emissions differences of the contributions of various source categories by state and pollutant.
   4. Bar plots of changes from the previous year to the current year (e.g., 2008 to 2011) NEI for various source categories and pollutants.
   5. Side-by-side pie charts of source category contributions by pollutant and region.

**EVALUATION OF METEOROLOGICAL MODELING RESULTS**

Overall Recommendations:

* Statistical and graphical comparisons that are partitioned into meaningful subsets, such as by observational site, geographic sub-regions, and daily/monthly/seasonal periods.
* Break out model performance aloft, at the surface, during individual episodes (e.g., high ozone / PM2.5 days), over the diurnal cycle, and as a function of synoptic regime.

Recommended statistical analyses:

1. For temperature, mixing ratio, wind speed and direction, and precipitation, calculate the values of the following statistics for each day and for monthly averages:
   1. Number of Data Points
   2. Mean Model / Observations
   3. Mean Bias / Error
   4. Fractional Bias / Error
   5. Correlation Coefficient
2. Where appropriate, calculate the same statistical outcomes (as above) for high pollution episodes for ozone and PM2.5.

Recommended graphical displays:

1. For temperature, mixing ratio, wind speed and direction, and precipitation generate:
   1. time-series plots of hourly modeled and observed data at individual monitor sites
   2. scatter plots of hourly modeled and observed data at individual monitor sites
   3. spatial plots of hourly modeled and observed data
   4. vertical profiles of modeled and observed data
   5. Q-Q plots of hourly modeled and observed data at individual monitor sites
   6. Box plots of hourly modeled and observed data at individual monitor sites
   7. Whisker plots of hourly modeled and observed data at individual monitor sites
2. Daily and/or monthly spatial plots of modeled and observed:
   1. cloud cover and precipitation
   2. observed albedo and snow depth for the winter season
3. Diurnal cycle plots of the model and observed planetary boundary layer height for time periods with measurements
4. Timeseries comparisons of modeled and observed shortwave downward radiation where available

**EVALUATION OF PHOTOCHEMICAL MODELING RESULTS**

Overall Recommendations:

* Pollutants: Ozone, NOX, NOY, VOC, speciated VOC, HNO3, NO, NO2, PAN, CO, CH4, SO2, NH3, total PM2.5, and speciated PM2.5 (SO4, NO3, NH4, elemental carbon, organic carbon, and crustal elements)
* Statistical analyses should be calculated for pollutants and time periods that are most relevant for understanding the processes important for a given model application.
  + - Averaging Period: Based on hourly averages and averages that correspond with the form of the air quality standard or metric being evaluated for each pollutant:
      * Ozone: hourly, maximum 8-hour average (MDA8), 60 ppb threshold
      * PM2.5: hourly and daily
    - Episode Selection: Screen results and limit number of days for which detailed analyses are needed for the report.
    - Monitoring Sites: Analyses of ozone and PM2.5 should be evaluated at individual monitoring sites based on hourly averages and averages that correspond with the form of the air quality standard.
* It may be valuable to aggregate certain regions (or even down to individual monitor) or time periods and evaluate model performance for those specific subsets:
  + - observational site
    - geographic sub-regions
    - daily/monthly/seasonal/diurnal time periods
    - vertical structure (aloft, surface)
    - synoptic regime (where applicable)

Recommended statistical analyses:

1. For each pollutant and averaging period listed above, calculate the values of the following statistics for each day and for monthly averages:
   1. Number of Data Points
   2. Mean Model / Observations
   3. Mean Bias / Error
   4. Normalized Mean Bias / Error
   5. Mean Fractional Bias / Error
   6. Correlation Coefficient

Recommended graphical displays (for each pollutant and averaging period listed above):

1. Time-series plots of modeled and observed at individual monitor sites.
2. Scatter plots of modeled and observed at individual monitor sites.
3. Spatial plots of modeled and observed across domain and subsets of domain to focus on certain/unique chemical and physical processes.
4. Vertical profiles of modeled and observed ozone for locations and time periods with aloft measurements (e.g., ozonesondes).
5. Q-Q plots of hourly modeled and observed data at individual monitor sites
6. Box plots of hourly modeled and observed data at individual monitor sites
7. Whisker plots of hourly modeled and observed data at individual monitor sites

Other recommended analyses:

1. Weekly spatial plots of modeled and observed data for NADP wet and CASTNet dry deposition.
2. Scatter plots of weekly and seasonal averages at individual monitor sites for wet deposition.
3. Plots of Indicator Ratios
4. Process Analysis: Emissions, Deposition, Advection, Diffusion, Vertical Mixing, and Net Change from Chemistry at various timesteps.

1. Note: Quality assurance checks for methane may depend on the completeness of the NEI for this constituent. [↑](#footnote-ref-2)
2. This analysis could consider Maximum Incremental Reactivity (MIR) values developed by William P. L. Carter. [↑](#footnote-ref-3)