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

**Statistical and Graphical Displays Checklist**

**ASSESSMENT OF BOUNDARY CONDITIONS**

* MPE plots, Wiki

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.

* MPE Plots: 2011 Base11a\_GCBC (includes various soccer, scatter, and timeseries plots)
* BC assessments were performed as part of 2011a MPE. See the wiki: [BC-Sensitivity-Modeling-Results](http://vibe.cira.colostate.edu/wiki/SiteSettings/Wiki/Index/1043?title=BC-Sensitivity-Modeling-Results). For example:
* √ Spatial Plots (Daily max O3 and BC sensitivity animations): Table 1
* √ Spatial Plots of BC tracers: Table 2
* √ Time Series: CAMx vs IMPROVE observations for sites in the 12km domain.
* √ BC curtain plots: Table 3 for O3, Ox, coarse and fine dust
* We don’t have plots available for speciated PM; please clarify what is meant by stratospheric intrusion and fires.
* We don’t have methane plots available, but we could create these; please clarify how CH4 applies to BC assessments

1. The analysis would focus on the boundaries and individual rural or remote sites.

* All of the products on the BC sensitivity wiki focus on these requirements

1. These types of plots will aid in identifying days on which the model has high background levels.
2. 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

* Emissions processing QA, MPE plots, ERT, Wiki

Recommended quality assurance activities:

1. Check inventory data codes to ensure they are valid codes.

* Please clarify what inventory data codes are

1. Compare post-SMOKE annual totals with Emissions Modeling Framework (EMF) inventory totals; usual tolerance is 1.0% or less

* √ Done (as part of emissions processing QA)

1. 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

* √ Done (as part of emissions processing QA)

1. Rank emissions and calculate percent differences with previous emissions estimates

* √ Wiki: *Modeling Platform*->Emissions Pages-> Emissions summaries-> modeling platform comparison (e.g. [Base 11a- Base 11b VOC](http://vibe.cira.colostate.edu/wiki/Attachments/Emissions/VOC_Base11b_vs_11a_Bar_RelDiff.png) for CO, UT, and WY)
* Note: Emissions are not ranked; relative difference is shown for some pollutants only
* √ ERT: emissions at the SCC level can be sorted by emissions magnitude.
* ERT modification: enable sorting by emissions magnitude on all tabular displays.
* ERT modification: plot differences in emissions between modeling platforms. (would need to account for any differences in emissions category mappings between platforms).

1. Compare previous emissions, new (or proposed) emissions, region-by-region emissions, and the computed difference or percent difference side-by-side.

* √ MPE Plots: Tile plots of monthly difference (Jan., June, July) by emissions category, chemical species, for 36km domain.
* e.g. 2011 Base11b -> EMIS -> Tileplots -> *36km* -> *emissions category* 🡪 monthly diff -> base11b-base11a -> *chemical species*
* Emissions GIS modification: county level emissions GIS prototype modified to allow selections at emissions category and SCC levels.

1. This analysis should be done one pollutant at a time for the following: analyzing NOx, VOCs, NH3, CH4,[[1]](#footnote-1) SO2, PM2.5, PM10, and PMC, and all source categories.

* √ Resources listed above include the major pollutants and source categories. The ERT and pie chart emissions GIS prototype are the only tools to show county level emissions at the SCC level (however ERT does not include PM10).

Recommended graphical displays:

1. Map emissions values for individual SCCs, groups of SCCs, county level emissions, and emissions differences among inventories

* √ MPE Plots: Tile plots of monthly total (Jan., June, July) by emissions category, chemical species, and modeling domain.
* e.g. 2011 Base11b -> EMIS -> Tileplots -> *(4km or 12km)* -> *emissions category* 🡪 monthly\_total -> *chemical species*
* Spatial emissions GIS prototype – (with modifications to display differences between inventories, and filter by emissions category and SCC).

1. Spatial plots with pie charts for each county of the various source category contributions by pollutant and region.

* Zac made this type of plot for the 2011a emissions, for a limited number of states/pollutants.
  + Wiki: 2011a modeling platform->SMOKE 2011a Emissions->Emissions Maps (e.g. [WY VOC](http://vibe.cira.colostate.edu/wiki/Attachments/Images/WY_AQ_3SAQS_B11a_VOC_Emissions.png))
* GIS development: Create a work flow to automate this in Arc Map; steps: 1) organize the emissions reports in a row/database flat format (maybe via a query from the ERT database; 2) import the report into ArcMap; 3) import other layers in to ArcMap (state/county boundaries, public land boundaries, roads, topography); 4) display thematic map by county with total emissions; 5) display pie charts for each county showing the distribution of emissions by sector

1. Bar plots of source category contributions by county by pollutant.

* √ ERT: Modeling Platform-> Pollutant-> Source Category-> State-> County (note: for any select box option, single or multiple selections are possible. Charts are organized so that each pollutant has a separate plot, each state is a separate bar in the plot (or each county if a single state is selected), and each source category is a component of each bar.
* √ Wiki: *Modeling Platform*->Emissions Pages-> Emissions summaries-> Stacked bar charts (e.g [2011b VOCs](http://vibe.cira.colostate.edu/wiki/Attachments/Emissions/2011b_VOC_Emissions_Stacked.png) by State and source category)

1. Tabulate the significant sources (SCC) contributing to each source category by pollutant and region.

* √ ERT – Modeling Platform-> Pollutant-> Source Category-> State-> County ->SCC (SCC contributions are displayed in a sortable table; Emissions at the SCC level are presented in a tabular display for a single county)

1. Pie Chart of Spatial, Temporal, and Chemical Allocations by source category by pollutant.

* Are these charts by profile assignments? Need clarification.

1. Bar, spatial, and pie plots of VOC Reactivity Analysis (RTOG/TOG)[[2]](#footnote-2) for various source category contributions by region.

* Need to have MIRs by speciation profile ID to do this. These data can be provided for one off analysis as needed
* Suggest building a page for VOC speciation analyses that could include profiles, cross-references, and MIR information

1. Plots and Tables of spatial and temporal allocations and chemical speciation assignments.

* This is analysis that can be done one off via reports provided by emissions modelers;
* We don’t have this information in the database right now to drive interactive tools. Is this something we want to pursue?

1. 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.

* ERT modification: - enable multiple modeling platform (emissions inventory) selection
* √ Wiki: See the 2008b, 2011a, and 2011b emissions wikis to see these charts. [Base 2011b Emissions Wiki](http://vibe.cira.colostate.edu/wiki/wiki/2078/waqs-2011b-platform-base-year-emissions) and scroll down to “Emissions Summaries”.
  1. Trends tables between years for various sectors and pollutants by region.
* ERT modification: display simple table showing trends for selected inventories
* See powerpoint for 2011a or 2008b emissions (examples?)
  1. Bar plots of emissions differences of the contributions of various source categories by state and pollutant.
* ERT - modified for multiple inventory selection
* √ Wiki: See the 2008b, 2011a, and 2011b emissions wikis to see these charts. . [Base 2011b Emissions Wiki](http://vibe.cira.colostate.edu/wiki/wiki/2078/waqs-2011b-platform-base-year-emissions) and scroll down to “Emissions Summaries”.
  1. Bar plots of changes from the previous year to the current year (e.g., 2008 to 2011) NEI for various source categories and pollutants.
* √ Wiki: See the 2011a emissions wiki
* 3SAQS emissions report and PPTs for these plots (examples?)
  1. Side-by-side pie charts of source category contributions by pollutant and region.
* See Section 4.2 the 3SAQS emissions modeling report from February 2015
* Development - spatial emissions GIS (modify to support two pie charts); ERT with multiple inventory selection

**EVALUATION OF METEOROLOGICAL MODELING RESULTS**

* MPE plots

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

* √ MPE plots: See AMET “Summary” plots for these stats under Plot browser (e.g. 2011 WRF -> ANNUAL\_BASE\_12km -> Summary-> ALL or *State*)
* √ MPE plots: See spatial\_surface plots for spatial plots of correlation coefficient, bias, mae, rmse for Q, T, WD, WS (e.g. 2011 WRF -> ANNUAL\_BASE\_12km -> spatial\_surface) (note: quite a few plots have no data)

1. 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

* √ MPE plots: hourly comparisons for each month averaged across states for Q, T, WS, WD for 4km domain (e.g. 2011 WRF -> ANNUAL\_BASE\_04km -> timeseries)
  1. scatter plots of hourly modeled and observed data at individual monitor sites
* √ MPE plots: see summary plots, above
  1. spatial plots of hourly modeled and observed data
  2. vertical profiles of modeled and observed data
  3. Q-Q plots of hourly modeled and observed data at individual monitor sites
  4. Box plots of hourly modeled and observed data at individual monitor sites
  5. Whisker plots of hourly modeled and observed data at individual monitor sites
* Don’t have any site-level plots for met; don’t have Q-Q, box, whisker, or vertical profiles for met; time series, scatter, spatial stats, and soccer plots are available on the plot browser

1. 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

* MPE plots: See plots for the winter O3 sensitivities; no obs for these

1. Diurnal cycle plots of the model and observed planetary boundary layer height for time periods with measurements

* Observed PBL heights are not readily available; need guidance

1. Timeseries comparisons of modeled and observed shortwave downward radiation where available

* Provide guidance on prioritization for this product

**EVALUATION OF PHOTOCHEMICAL MODELING RESULTS**

* MPE plots; Model-to-obs tool (MTO), SA visualization tool

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)
* Note – some chemical species do not have observations
* 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
* √ SA visualization tool (shows model-to-obs for 10 day period of MDA8 O3).
  + 2008b SA tool: <http://views.cira.colostate.edu/TSDW/Tools/SourceApportionment.aspx>
  + 2011a R1 SA tool: <http://vibe.cira.colostate.edu/WAQSSourceApp/>
* √ Interactive SA spreadsheets show annual modeled O3 timeline and allow superimposition of arbitrary (user defined) threshold value.
* MTO modification – calculate stats based on selected site/pollutant/metric/time range (currently tabular data show daily model-to-obs difference.)
  + - * PM2.5: hourly and daily
* √ MTO shows hourly or daily depending on monitoring network
  + - Episode Selection: Screen results and limit number of days for which detailed analyses are needed for the report.
* √ MTO (user can select any date range for display)
  + - 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.
* MPE plots:
* √ MTO for various species and metrics depending on obs network.
  + AQS – daily: O3 1& 8hr max, PM25, W126 (9cell aggregations not working)
  + AQS – hourly: gas phase species & PM25\_TOT (what is PM25\_TOT?)
  + CASTNet – daily: O3 1 & 8hr max (is the daily/hourly distinction for CASTNet and AQS a product of post processing data aggregation?)
  + CASTNet – hourly: hourly O3
  + CASTNet – weekly: speciated PM2.5 and PMTOT
  + CSN - daily: speciated PM2.5 and PMTOT
  + IMPROVE - daily : hourly average O3, PM2.5, speciated PM2.5, PMTOT (should replace “daily” with every third day
  + NADP – weekly: NH4, NO3, SO4 conc & dep (not working for 2008 data)
  + NAPS – hourly: (works for network comparison, not working for sites)
* 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
* √ MPE plots: timeseries (B11b.*network.species*.\*\*) compares obs with 11a &11b
  + \*\*All.All.ann.timeseries.png
  + \*\*.*Site.State*.ann.timeseries.png (all sites in *State* are in image set)
* √ MTO - compares network mean with obs mean, or single site with obs
  + - geographic sub-regions
* √ MPE plots: soccer plots by state. 2011 Base11b->AQ->4km->4km domain or *State*
* MTO modification – develop UI to select sub-regions and dynamically aggregate model and obs values based on selection.
  + - daily/monthly/seasonal/diurnal time periods
* √ MPE plots: daily for timeseries, monthly for state soccer, box plots (diurnal-hourly), monthly (box and whisker). Other plot types include qq, ecdf, taylor, barplot.
* MTO modification – add additional time period filters and plot types
  + - 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

* For monthly average stats see the outstate files under: /mnt/data2/3SDW/3SAQS/2011/Base11b/AMET
  + Prototype tool: <http://views.cira.colostate.edu/TSDW/modeling/mpemetrics.aspx>

Tool provides tabular display of MPE metrics sortable across state and 4 or 12 km domain average (note: add n, model & obs mean to metrics). Do we want to add site level metrics?

* √ MPE plots – scatterplots: text box with summary stats for n, NMB, NME, FB, FE (note: add n, model & obs mean)
* √ MPE plots – soccer plots: graphical display of NME vs NMB (all, 04k\_Domain, *State*)
  + \*\*.ann.soccerplot.png - (e.g. 4km AQS year plot shows data point for each mo.
  + \*\*.*season*.soccerplot.png
  + \*\*.*month*.soccerplot.png – data points in 6 states for individual month B11a & B11b
  1. Mean Fractional Bias / Error
  2. Correlation Coefficient
* √ MPE plots: statsplots for each pollutant (FB, FE, ME, NMB, NME, RMSE, Corr) in 4km domain
* MTO modification – Calculate tabular statistics on-the-fly based on user defined monitoring site selection. Recreate certain chart types currently created using AMET…

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

1. Time-series plots of modeled and observed at individual monitor sites.

* √ MTO: compares monitoring site obs with appropriately aggregated model output. (could add bias plot output to match AMET generated graphics)
* √ MPE plots - timeseries plots (show 11a & 11b and obs, panel 1 magnitude, panel 2 bias from obs)

1. Scatter plots of modeled and observed at individual monitor sites.

* √ MPE plots: scatterplots, (e.g. Base11b->AQ->4km->all (04km\_Domain, *State*) (note image name and path do not indicate obs network(s) for scatterplots because there may be obs from two networks represented)
  + \*\*.ann.scatterplot.png
  + \*\*.*season*.scatterplot.png
  + \*\*.*month*.scatterplot.png

1. Spatial plots of modeled and observed across domain and subsets of domain to focus on certain/unique chemical and physical processes.

* √ MPE plots (Created with PAVE, AQ->4km->04km\_domain-> network)

1. Vertical profiles of modeled and observed ozone for locations and time periods with aloft measurements (e.g., ozonesondes).

* Don’t have for 2008, 2011. Check 2011a MPE Report.

1. Q-Q plots of hourly modeled and observed data at individual monitor sites

* √ MPE plots – annual qq for each pollutant, model vs obs; plots show 11a and 11b

1. Box plots of hourly modeled and observed data at individual monitor sites

* √ MPE Plots: Hourly, diurnal, day of the week

1. Whisker plots of hourly modeled and observed data at individual monitor sites

* √ MPE plots: 11b->AQ->4km->*State* monthly box and whisker plots for obs, 11a, 11b

Other recommended analyses:

1. Weekly spatial plots of modeled and observed data for NADP wet and CASTNet dry deposition.

* Don’t have spatial plots for deposition (other than stats plots, see below)

1. Scatter plots of weekly and seasonal averages at individual monitor sites for wet deposition.

* √ MPE plots: some “network” scatter plots include NADP (e.g. 2011 Base11b->AQ->12km->12k\_Domain (see parameter.region SO4\_dep.All). This appears to be the only 12km NADP scatter plot.
* √ MPE plots: NAPD annual stats plots (e.g. 2011 Base11b->AQ->4km->04k\_Domain (see parameters.region NH4\_dep.All, NO3\_dep.All, SO4\_dep.All). Site level time series (e.g. 2011 Base11b->AQ->4km->*State*, see parameter NH4\_dep, NO3\_dep, etc.)
* √ MPE plots: CASTNet timeseries and soccer plots (e.g. 2011 Base11b->AQ->4km->all (see network parameters.region CASTNET\_drydep.HNO3\_ddep.All, *State*,04k\_Domain, NH4\_ddep, NO3\_ddep, SO2\_ddep, TNO3\_ddep). Time series are only for All.
* √ MTO: NADP-weekly - wet dep comparisons for NH4, NO3, SO4 averaged across network (site level comparisons not working) CASTNet dry dep values are not compared to model because CASTNet reports dry deposition using climatological average deposition flux.
* MTO modification: ability to aggregate NADP plots by season

1. Plots of Indicator Ratios

* Not available

1. Process Analysis: Emissions, Deposition, Advection, Diffusion, Vertical Mixing, and Net Change from Chemistry at various timesteps.

* Not available

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