

Model Performance Statistics and Graphics

1. Methods:

- Pollutants:
 - Pollutant definitions (all species are explicitly modeled and measured unless otherwise noted). Note that fine particle modes in CMAQ have been defined as the sum of Aitken (i) and accumulation (j) modes.
 - Al - fine particulate aluminum
 - CO - carbon monoxide
 - Ca - fine particulate calcium
 - Cl – fine particulate chloride
 - EC¹ – fine particulate elemental carbon
 - Fe – fine particulate iron
 - HNO₃ – nitric acid
 - K – fine particulate potassium
 - Mg – fine particulate magnesium
 - Mn – fine particulate manganese
 - Na – fine particulate sodium
 - NaCl - fine particulate sodium chloride = Na + Cl
 - NCOM – fine particulate non-carbon organic matter
 - CMAQ = OM - OC
 - CAMx = OM - OC
 - Observations = 0.8 × OC
 - NH₄² – fine particulate ammonium
 - NO – nitric oxide
 - NO₂ – nitrogen dioxide
 - NO₃³ – fine particulate nitrate
 - NOX = NO + NO₂
 - NOY – total reactive nitrogen
 - CMAQ = NO + NO₂ + NO₃ (gas) + 2×N₂O₅ + HONO + HNO₃ + PNA + CRON + CLNO₂ + PAN + PANX + OPAN + NTR1 + NTR2 + INTR + NO₃ (particle)
 - CAMx = NO + NO₂ + NO₃ (gas) + 2×N₂O₅ + HONO + HNO₃ + PNA + CRON + CLNO₂ + PAN + PANX + OPAN + NTR1 + NTR2 + INTR + NO₃ (particle)
 - O₃ = O₃_hourly – hourly ozone (all hours)
 - O₃_1hrmax – 1-hr daily maximum ozone (MDA1)

¹Graphics for EC may also appear in a PM25_EC directory for some annual plots

²Graphics for NH₄ may also appear in a PM25_NH₄ directory for some annual plots

³Graphics for NO₃ may also appear in a PM25_NO₃ directory for some annual plots

- O3_1hrmax_bysite – 1-hr daily maximum (MDA1) ozone for site-level timeseries
- O3_8hrmax - 8-hr daily maximum (MDA8) ozone
- O3_8hrmax_GE60 – 8-hr daily maximum (MDA8) ozone at sites/days with measured ozone greater than 60 ppb
- O3_8hrmax_bysite – 8-hr daily maximum (MDA8) ozone for site-level timeseries
- OC⁴ – fine particulate organic carbon
- Other – unspiciated PM including NCOM
 - OBS = PM2.5 – (SO4+NO3+NH4+OC+Ca+Na+Cl+Soil)
 - CMAQ = PM2.5 – (SO4+NO3+NH4+OC+Ca+Na+Cl+Soil)
 - CAMx = PM2.5 – (SO4+NO3+NH4+OC+Ca+Na+Cl+Soil)
- Other_rem – unspiciated PM excluding NCOM
 - OBS = PM2.5 – (SO4+NO3+NH4+1.8×OC+Ca+Na+Cl+Soil)
 - CMAQ = PM2.5 – (SO4+NO3+NH4+OC+NCOM+Ca+Na+Cl+Soil)
 - CAMx = PM2.5 – (SO4+NO3+NH4+OC+Ca+NCOM+Na+Cl+Soil)
- PM_TOT⁵ – fine particulate matter
 - CMAQ and CAMx = sum of all fine particulate species
 - Observations = PM mass measured by FRM, FEM (11 different methods at AQS sites) and similarly performing methods
- SO2 – sulfur dioxide
- SO4⁶ – fine particulate sulfate
- Si – fine particulate silicon
- Soil⁷ – calculated soil mass as defined by the IMPROVE monitoring network
 - $2.2 \times \text{Al} + 2.49 \times \text{Si} + 1.63 \times \text{Ca} + 2.42 \times \text{Fe} + 1.94 \times \text{Ti}$
- TC – total carbon = OC + EC
- TNO3 – total nitrate = nitric acid + fine particulate nitrate
- Ti – fine particulate titanium
- Temporal average of measurements
 - The following pollutants are measured as hourly averages: O3, CO, NO, NO2, NOX, NOY, SO2, PM_TOT (some AQS sites).
 - The following pollutants are measured as 24-hour averages: Al, Ca, Cl, EC, Fe, HNO3, K, Mg, Mn, NH4, NO3, Na, NaCl, OC, SO4, Si, TC, TNO3, Ti, NCOM, Other, soil, PM_TOT (CSN, IMPROVE, and some AQS sites).

⁴ Graphics for OC may also appear in a PM25_OC directory for some annual plots

⁵ Graphics for PM_TOT may also appear in a PM25 directory for some annual plots

⁶ Graphics for SO4 may also appear in a PM25_SO4 directory for some annual plots

⁷ Graphics for Soil may also appear in a PM25_SOIL directory for some annual plots

- PM_TOT is measured on an hourly average at some sites and as 24-hr averages at other sites. AQS_Hourly network data includes all hourly measurements. AQS_Daily network data includes both 24-hr average measurements and hourly data aggregated up to 24-hr averages.
 - Daily ozone values for MDA8, MDA1, MDA8_GE60 are also calculated from hourly ozone data.
 - Modeled and observed values are paired in space and time
 - Modeled values in the grid-cell whose center is closest to the monitor are paired with the observed values at the monitor
 - Modeled hourly values are aggregated up to the time interval of the measurements (i.e. 24 hours for filter-based gravimetric PM measurements)
 - Hourly modeled and observed ozone values are also used to calculate daily maximum 1-hr daily (MDA1) ozone and daily maximum 8-hr (MDA8) ozone. MDA8 ozone is calculated using methods described in 40 CFR Appendix P to part 50. Note that the modeled and observed MDA8 values may be based on different sets of hours.
 - Model layer 1 (L1) is 20m thick and the predictions represent layer-average concentrations. Pairing of model L1 values with observed values at monitors which sample air 3-10m above the ground, does not account for any vertical gradients that affect measured concentrations but are not explicitly simulated in the model.
 - A range of statistics are calculated using observed and predicted data pairs for monitoring sites within each NOAA climate region (Figure 1) and for each season (Spr = MAM, Sum = JJA, Fall = SON, Win = DJF). MDA8 ozone statistics are reported both on all days and on days when observations are above 60 ppb.
 - These statistics represent both a temporal and spatial aspects since you include multiple days of data per site and data collected at multiple sites per region.
 - Data completeness criteria of 75% are applied.
 - Standard metrics used in model performance evaluations are defined in Table 1

Table 1: standard model performance metric definitions

Abbreviation	Statistic Name	Formula	Units
n	Number of obs		--
--	Observed Mean	$\frac{1}{n} \sum_{i=1}^n O$	ppb or $\mu\text{g}/\text{m}^3$
--	Modeled Mean	$\frac{1}{n} \sum_{i=1}^n M$	ppb or $\mu\text{g}/\text{m}^3$
MB	Mean Bias	$\frac{1}{n} \sum_{i=1}^n M - O$	ppb or $\mu\text{g}/\text{m}^3$
ME	Mean Error	$\frac{1}{n} \sum_{i=1}^n M - O $	ppb or $\mu\text{g}/\text{m}^3$
RMSE	Root Mean Square Error	$\sqrt{\frac{\sum_{i=1}^n (M - O)^2}{n}}$	ppb or $\mu\text{g}/\text{m}^3$
NMB	Normalized Mean Bias	$100 \times \frac{\sum_{i=1}^n (M - O)}{\sum_{i=1}^n O}$	%
NME	Normalized Mean Error	$100 \times \frac{\sum_{i=1}^n M - O }{\sum_{i=1}^n O}$	%
FB	Fractional Bias	$100 \times \frac{1}{n} \left(\frac{\sum_{i=1}^n (M - O)}{\sum_{i=1}^n \frac{M + O}{2}} \right)$	%
FE	Fractional Error	$100 \times \frac{1}{n} \left(\frac{\sum_{i=1}^n M - O }{\sum_{i=1}^n \frac{M + O}{2}} \right)$	%
r	Correlation	$\frac{1}{n-1} \sum_{i=1}^n \left(\left(\frac{O - \bar{O}}{\sigma_O} \right) \times \left(\frac{M - \bar{M}}{\sigma_M} \right) \right)$	--

M = predicted concentration, O = observed concentration, σ = standard deviation

U.S. Climate Regions

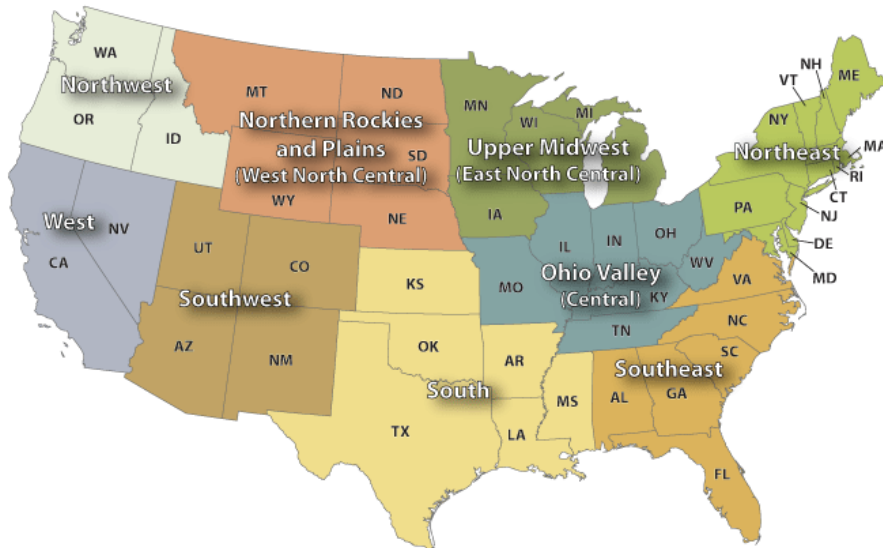


Figure 1. NOAA climate regions (source: <https://www.ncdc.noaa.gov/monitoring-references/maps/us-climate-regions.php>)

2. Naming and Organization of Model Performance Graphics

- File naming convention: MODELVERSION_POLLUTANT_NETWORK_PLOTTYPE.png/html
 - MODELVERSION = CMAQ_2016ff_12US2 or CAMx_2016ff_12US2. In graphics which include data from both model simulations, both MODELVERSIONS are included in the file name.
 - POLLUTANT names are defined in section 1.
 - NETWORK = AQS_Hourly, AQS_Daily, CSN, IMPROVE, CASTNET, NADP or multi_network
 - PLOTTYPE names provided in sections 3 and 4.
- Directory structure for graphics (separate directory structures exist for static MPE graphics and interactive html graphics)
 - Region (9 NOAA regions + National = 10 regions). National directory includes national maps and tile “Kelly” plots which show statistics for all regions.
 - Season (4 seasons + Annual = 5 seasons). Annual directory includes 1) boxplots that show temporal distribution of data throughout the year, 2) tile “Kelly” plots that show statistics for all four seasons, 3) daily plots for each day of the year and 4) visibility plots that show data on 20% observed clearest and 20% observed most impaired days.
 - Pollutant
- Graphics located in National/Annual directory
 - Statistical tile “Kelly” plots
 - Visibility plots for 20% clearest and 20% most impaired days at each IMPROVE site
 - Monthly average model-model difference national maps for
- Graphics located in National/Season directories
 - National/seasonal network statistics maps for concentration and deposition.
- Graphics located in Region/Annual directories
 - Daily model-obs overlay regional maps for each day of the year
 - Daily model-model difference regional maps for each day of the year
 - Regional/monthly boxplots
- All other graphics located in Region/Season directories

3. Description Static MPE Graphics

- National statistical tile “Kelly” plot:
 - Naming convention for these plots:
Tile_POLLUTANT_METRIC_NETWORK_MODELVERSION
 - MODELVERSION = 2016ff_CMAQ or 2016ff_CAMx
 - METRIC = Correlation, Mean Bias, Percent_Norm_Mean_Bias, or RMSE
 - Statistics are calculated using equations in Table 1. Calculations use all site-day/hour combinations for each region and season.
 - The color on any particular tile represents the value of the metric for a specific region and season combination.
- National/seasonal network statistics map: PLOTTYPE = “stats_map_METRIC”
 - Displaying statistics at individual monitoring sites calculated using equations in Table 1. Calculations use all hours or days at each site.
- Regional/seasonal network statistics map
 - Same as the national/seasonal network statistics map except only includes data for a single NOAA climate region
- National maps of monthly CMAQ/CAMx differences:
 - Naming convention for these plots:
CMAQ_CAMx_2016ff_POLLUTANT_NETWORK_PLOTTYPE_MM.png
 - PLOTTYPE = “mod_mod_diff_map”
 - MM = month
 - Top-left panel shows gridded monthly average CMAQ concentrations (ppb or $\mu\text{g}/\text{m}^3$)
 - Top-right panel shows gridded monthly average CAMx concentrations (ppb or $\mu\text{g}/\text{m}^3$)
 - Bottom-left panel shows gridded absolute CMAQ-CAMx difference (ppb or $\mu\text{g}/\text{m}^3$) in monthly average concentrations
 - Bottom-right panel shows gridded percent CMAQ-CAMx difference in monthly average concentrations
- Regional maps of daily CMAQ/CAMx model differences:
 - Naming convention for these plots:
CMAQ_CAMX_2016ff_POLLUTANT_NETWORK_PLOTTYPE_MM.DD.pnt
 - PLOTTYPE = “daily_modmod_diff_map”, date appears at end of filenames in MM.DD form.
 - Top-left panel shows gridded daily CMAQ concentrations (ppb or $\mu\text{g}/\text{m}^3$)
 - Top-right panel shows gridded daily CAMx concentrations (ppb or $\mu\text{g}/\text{m}^3$)
 - Bottom-left panel shows gridded absolute daily CMAQ-CAMx difference (ppb or $\mu\text{g}/\text{m}^3$)
 - Bottom-right panel shows gridded daily percent CMAQ-CAMx difference

- Regional model-obs overlay plot
 - Naming convention for these plots:
PROJECT_POLLUTANT_NETWORK_PLOTTYPE_MM.DD.png
 - PLOTTYPE = “daily_obs_overlay_map”
 - Left panel shows daily gridded fields of model concentrations with overlaid observed values at monitor locations
 - Right panel shows difference between modeled values and observed values at monitor locations (Model – Observation)
- Regional/monthly boxplots: PLOTTYPE – “boxplot_all”; “boxplot_bias”, “boxplot_norm_bias”
 - boxplot_all: Distribution of observed, CMAQ, and CAMx pollutant concentration by month. Boxes represent interquartile range and centerlines represent median values.
 - boxplot_bias and boxplot_norm_bias: Distribution of CMAQ and CAMx bias/NMB by month. Boxes represent interquartile range and centerlines represent median values.
- Regional/seasonal timeseries: PLOTTYPE – “timeseries”
 - Regional mean Obs and Model concentrations by day along with daily bias, RMSE and correlation calculated using equations in Table 1 across all site and day combinations. Note that for “bysite” time series the correlation will always be 0 because the sample size for each timestep = 1.
- Regional/seasonal binned scatterplot: PLOTTYPE – “scatterplot_bins”
 - Distribution of mean bias (left panel) and RMSE (right panel) binned by observed concentration ranges. Whiskers indicate interquartile range, triangles indicate median values and asterisks indicate mean values. The number of site and day combinations within each observation-based concentration bin are shown at the bottom of the plot.
- Regional/Seasonal density scatterplot: PLOTTYPE – “scatterplot_density”
 - Scatterplot of modeled concentrations (y-axis) versus observed concentrations (x-axis).
 - The plotting area is broken down into small bins (1 ppb X 1 ppb for ozone) and the color represents the percent of total datapoints (site and day combinations) that fall in a specific location of the plotting area. Therefore, warmer colors show locations that represent a larger fraction of the datapoints.
 - These plots are good for visualizing scatterplots in cases where there are large numbers of overlapping datapoints.
 - The dotted line and the formula in the upper left corner represent the line-of-best-fit for the data using ordinary least squares regression.
- Regional/Seasonal density scatterplot ggplot: PLOTTYPE – “scatterplot_density_ggplot”

- Scatterplot of modeled concentrations (y-axis) versus observed concentrations (x-axis).
- The plotting area is broken down into small bins and the color represents the number of datapoints (site and day combinations) that fall in a specific location of the plotting area. Therefore, warmer colors show locations that represent a larger fraction of the datapoints.
- These plots are good for visualizing scatterplots in cases where there are large numbers of overlapping datapoints.
- The solid line represents the one-to-one line for modeled versus observed concentrations
- The dotted line and the formula in the upper left corner represent the line-of-best-fit for the data using ordinary least squares regression.
- The gray shaded area shows the 95% confidence interval around the line-of-best-fit.
- Regional/seasonal skill scatterplot: PLOTTYPE – “scatterplot_skill”
 - Scatterplot of modeled concentrations (y-axis) versus observed concentrations (x-axis).
 - Plot is split into 4 quadrants based modeled/observed values above and below 70 ppb. Numbers printed in the corner of each quadrant show the number of datapoints.
 - Q1 (model > 70, obs > 70) represents site/days when the model correctly predicted MDA8 ozone values > 70 ppb.
 - Q2 (model < 70, obs > 70) represent site/days when the model incorrectly predicted that MDA8 ozone would be < 70 ppb (“misses”)
 - Q3 (model < 70, obs < 70) represent site/days when the model correctly predicted that MDA8 ozone < 70
 - Q4 (model > 70, obs < 70) represents site/days when the model incorrectly predicted MDA8 ozone < 70 (“false alarms”)
- Visibility plots:
 - Located in 2 pollutant directories. Each directory contains one plot for every IMPROVE monitoring site.
 - VISIBILITY_CONC = stacked barplots of PM species composition ($\mu\text{g}/\text{m}^3$) on the 20% clearest and 20% most impaired days
 - VISIBILITY_EXT = stacked barplots of PM species extinction (Mm^{-1}) calculations on the 20% clearest and 20% most impaired days
 - Observations of composition and extinction were obtained from the IMPROVE monitoring network dataset¹
 - Extinction and speciated PM composition are calculated using the second IMPROVE algorithm as detailed at: <http://vista.cira.colostate.edu/Improve/the-improve-algorithm/>
 - $b_{\text{ext}} \approx 2.2 \times f_s(\text{RH}) \times [\text{Small Ammonium Sulfate}] + 4.8 \times f_l(\text{RH}) \times [\text{Large Ammonium Sulfate}] + 2.4 \times f_s(\text{RH}) \times [\text{Small Ammonium Nitrate}] + 5.1 \times f_l(\text{RH})$

$\times [Large\ Ammonium\ Nitrate] + 2.8 \times [Small\ Organic\ Mass] + 6.1 \times [Large\ Organic\ Mass] + 10 \times [Elemental\ Carbon] + 1 \times [Fine\ Soil] + 1.7 \times f_{ss}(RH) \times [Sea\ Salt] + 0.6 \times [Coarse\ Mass] + Rayleigh\ Scattering\ (Site\ Specific)$

- $f_s(RH)$, $f_L(RH)$, and $f_{ss}(RH)$ are water growth terms which are functions of relative humidity. The values used in the calculation of day/site specific extinction are pre-calculated site-specific monthly climatological $f(RH)$ data obtained from the IMPROVE monitoring network dataset.⁸ The same values are used in both the observed and modeled extinction calculations.
- *Rayleigh Scattering (Site Specific)* values used in the calculation of day/site specific extinction are obtained from the IMPROVE monitoring network dataset¹
- Note that, consistent with the IMPROVE data procedures, values for ammonium sulfate, ammonium nitrate, organic mass, and soil were calculated both for the observations and for the model data. For instance, organic mass was calculated using the 1.8 multiplier times modeled OC rather than the modeled total organic mass.
- *Ammonium sulfate = 1.375 × sulfate*

Large Ammonium Sulfate

$$= \begin{cases} \text{if ammonium sulfate} \geq 20, \text{ then ammonium sulfate} \\ \text{if ammonium sulfate} \leq 20, \text{ then } \frac{\text{ammonium sulfate}^2}{20} \end{cases}$$

- *Small Ammonium Sulfate = ammonium sulfate – large ammonium sulfate*

- *Ammonium nitrate = 1.29 × nitrate*

- Large Ammonium Nitrate =

$$\begin{cases} \text{if ammonium nitrate} \geq 20, \text{ then ammonium nitrate} \\ \text{if ammonium nitrate} \leq 20, \text{ then } \frac{\text{ammonium nitrate}^2}{20} \end{cases}$$

- *Small Ammonium nitrate = ammonium sulfate – large ammonium nitrate*

- *Organic mass = 1.8 × OC*

- Large Organic Mass =

$$\begin{cases} \text{if organic mass} \geq 20, \text{ then organic mass} \\ \text{if organic mass} \leq 20, \text{ then } \frac{\text{organic mass}^2}{20} \end{cases}$$

- *Small Organic mass = Organic Mass – large organic mass*

- *Fine Soil = 2.2 × Al + 2.49 × Si + 1.63 × Ca + 2.42 × Fe + 1.94 × Ti*

- In the stacked barplot, *bext* is split out by species such that $bext_sulfate = 2.2 \times f_s(RH) \times [Small\ Ammonium\ Sulfate] + 4.8 \times f_L(RH) \times [Large\ Ammonium\ Sulfate]$; $bext_nitrate = f_s(RH) \times [Small\ Ammonium\ Nitrate] + 5.1 \times f_L(RH) \times$

⁸

http://vista.cira.colostate.edu/DataWarehouse/IMPROVE/Data/SummaryData/RHR_2017/sia_impairment_daily_budgets_10_18.csv

$[Large\ Ammonium\ Nitrate]$, $bext_organic = 2.8 \times [Small\ Organic\ Mass] + 6.1 \times [Large\ Organic\ Mass]$; $bext_elementalcarbon = 10 \times [Elemental\ Carbon]$;
 $bext_soil = 1 \times [Fine\ Soil]$; $bext_seasalt = 1.7 \times f_{ss}(RH) \times [Sea\ Salt]$;
 $bext_coarsemass = 0.6 \times [Coarse\ Mass]$

- Each plot has a panel for the 20% Most Impaired days and a panel for the 20% Clearest days according the method documented in Gantt et al. (2018)⁹ and in US EPA (2018)¹⁰. Assignment of days, both model and observed, is based on the observations.

4. Description of Interactive html Graphics

- National/seasonal network statistic map: PLOTTYPE = “stats_map_METRIC”
 - Display statistics by site using same information from the static National/seasonal network statistics map (“stats_map_METRIC”), but also includes the capability to query statistics, zoom-in, and underlay different basemaps.
- Regional/seasonal network statistics map
 - Display statistics by site using same information from the static image “stats_map_METRIC” png figures, but also includes the capability to query statistics, zoom-in, and underlay different basemaps.
- Regional/seasonal daily boxplot: PLOTTYPE = “boxplot”
 - Shows distribution of daily modeled and observed concentrations
 - Provides ability to turn on and off each set of boxplots by clicking on the legend symbol, to query date + values on any day by mousing over boxplot and to zoom in on any region of the plot by highlighting the box of interest with the mouse
 - Boxes represent interquartile range
 - Whiskers represent 1.5×interquartile range
 - Solid horizontal line within each box represents median value
 - Dashed horizontal line within each box represents mean value
 - Dashed triangles within each box represent +/- one standard deviation extending from the mean line
- Regional/seasonal daily timeseries: PLOTTYPE = “Daily_timeseries”
 - Plot provides timeseries of
 - Observed concentrations averaged across sites in the region
 - Modeled concentration averaged across sites in the region
 - Average model bias calculated as the difference between average obs and average mod

⁹ <https://www.tandfonline.com/doi/pdf/10.1080/10962247.2018.1424058>

¹⁰ https://www.epa.gov/sites/production/files/2018-12/documents/technical_guidance_tracking_visibility_progress.pdf

- Average RMSE calculated using the equation in Table 1 in which each site and day represent a separate datapoint (i.e. $n = \# \text{ sites} \times \# \text{ time steps}$)
 - Spatial correlation between observed and modeled concentrations
 - Interactive interface allows the user to turn on and off each timeseries line by clicking on the legend symbol, mouse over time series to query values at a specific times and control the zoom on the x- and y-axes.
- Site-specific daily timeseries: PLOTTYPE = "timeseries"
 - Plot provides timeseries of
 - Observed concentrations at the single monitoring site
 - Modeled concentration at the single monitoring site
 - Model bias at the single monitoring site
 - RMSE at the single monitoring site
 - Interactive interface allows the user to turn on and off each timeseries line by clicking on the legend symbol, mouse over time series to query values at a specific times and control the zoom on the x- and y-axes.