Intermountain Data Warehouse (IWDW)

Western Air Quality Study (WAQS)

Model Performance Efforts

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2017 Western Modelers Workshop

September 6 – September 8

OVERVIEW: IWDW – WAQS

Purpose of Study:

- Multiple federal and state agencies identified need to more efficiently collect air quality (AQ) data and conduct modeling to assess expanding number of oil and gas development.

Memorandum of Understanding (MOU):

- 2011: Pilot Study called Three State Air Quality Study (3SAQS)
- 2014: Extended MOU to continue efforts (IWDW – WAQS)

Benefits of Study:

- Centralized platform to store, share, and visualize data air quality data
- Prevents duplication of efforts for NEPA, SIP/FIP, and Planning Projects
- **Streamlines process to reduce uncertainty, time (1-2 years), and expense ($300K-$800K) of starting AQ analysis. Provides: Model Inputs for Baseline; No-Action Scenario, & Baseline MPE**

Products and Operations:

- **Monitoring:** Ozone and Particulate Matter Monitors
- **Modeling:** Emissions, Meteorology, Air Quality Modeling
  - **2008 Platform:** MOZART IC/BC; 2008/2020 Emissions; WRF; CAMx
  - **2011 Platform:** MOZART/Geos-Chem IC/BC; 2011/2020 Emissions; WRF; CAMx/CMAQ
- **Data Warehouse**: Air quality data and files (internal/external to Cooperators) related to monitoring, emission inventories, meteorology, air quality modeling. Visualization tools.

WAQS: PGM MPE Checklist

Purpose:

- Recommends series of model evaluation analyses for determining adequacy of PGM platforms
- Recommends approach for summarizing and interpreting MPE results
- Assists in identifying resources (time, funding, evaluation tools) needed to complete future MPEs

Background:

- **Builds upon EPA MPE guidance and supplemented with analyses relevant to western U.S. AQ**
- **Operational Evaluation:** Determine how well model replicates observed pollutant concentrations and deposition. Most modeling efforts focus on operational evaluations.
- **Diagnostic Evaluation:** Determine whether model accurately represents processes (emissions, meteorology, chemical reactions, deposition) impacting pollutant concentrations, and provide insights into causes of poor model performance. Conducted when sufficient resources exist.
- **Dynamic Evaluation:** Determine whether model can capture dynamic responses and long-term trends observed by monitors. Lack modeling results for long-term comparisons ($\leq$ 3 years).

Components of Checklist (in order of completion):

- Assessment of boundary conditions
- Evaluation of meteorological modeling results
- Assessment of emissions inventory and modeling results
- Evaluation of photochemical grid modeling results
- Summarizing and interpreting results of platform MPE

Assessment of Boundary Conditions

Purpose:

- Understand ability of Global Models (GM) to simulate transport of air pollution from outside domain, and identify days with large boundary contributions resulting from long-range or international transport, stratospheric intrusions, fires, or methane.

Initial Assessment Approach Options:

- **Evaluation of Global Model:** Review MPE completed by GM developers.
- **Lateral Boundary Inflow using Inert Simulation:** Simulation using BC inputs without emissions or chemistry. Minimal resources needed to complete this evaluation.

Additional Assessment using Base Platform:

- **Lateral Boundary Inflow using Reactive Tracer Simulation:** Simulation tracking BC inputs with reactive tracers to account for atmospheric chemistry (CAMx OSAT/PSAT, and CMAQ ISAM).
- **US Background Contribution using Chemistry Simulation:** Simulation with chemistry and no US anthropogenic emissions to assess US background levels of ozone and $PM_{2.5}$.
- **Full PGM Simulation:** Simulation with full-chemistry and emissions. Evaluation would focus on rural or remote sites that have little influence from US anthropogenic emissions.
- **Global Model Sensitivity:** Simulation with boundary inputs derived from different GMs. Evaluation should consider both performance aloft (ozone transport is most important), and surface comparisons.

Assessment of Meteorological Modeling

Purpose:

- Determine if model results represent a reasonable approximation of actual meteorology.
- Evaluate each day to identify days with good or poor model performance.

Parameters to Evaluate (impacts photolysis rates & formation of O_3):

- Temperature, mixing ratio, wind speed and direction
- Cloud cover and precipitation: Emerging dataset to consider includes the Parameter-elevation Relationships on Independent Slopes Model (PRISM).
- Albedo and snow depth for the winter season
- Planetary boundary layer height
- Shortwave downward radiation where available (SURFRAD and ISIS networks)

Recommended Analysis Approach:

- Evaluate performance aloft, at surface, during individual episodes (e.g., high ozone / $PM_{2.5}$ days), over diurnal cycle, and as a function of synoptic regime.
- Evaluate results against independent datasets not used in nudging analysis.

Diagnostic Evaluation:

- Different configuration options in iterative approach: Cumulus parameterization; Planetary Boundary Layer; Nudging alterations; Land Surface Model; Radiation; Microphysics

Assessment of Emissions Inventory

Purpose:

- Given that emission inventories (EIs) are compiled from multiple datasets, review EIs using Quality assurance (QA) checks to identify data problems (errors in emissions amounts, codes, facility names, stack heights, or latitude/longitude locations).

Recommended Quality Assurance Checks:

- **Checking data codes**: Ensure inventory codes are valid
- **Point versus nonpoint reconciliation:** Ensure sources are identified properly, are not double-counted across point and nonpoint, and do not have missing pollutant emission rates, temporal allocations or spatial components.
- **Rankings and percent differences techniques:** Rank emissions and calculate percent differences (with previous emissions estimates). Large or unexpected differences can be investigated further to ensure that differences have reasonable explanation.
- **Comparisons among emissions inventories and regions:** Use spatial plots and county and states totals to compare previous emissions, proposed emissions, region-by-region emissions, and the computed difference to reveal unexpected changes or patterns that could signal an error.

Additional Analyses:

- Evaluate VOC speciation by source category to determine if the emissions accurately represent the reactivity of the VOC mixture.

Assessment of PGM Platform

Purpose:

- Determine how well air quality model replicates observed concentrations of ozone, ozone precursors, total $PM_{2.5}$, individual $PM_{2.5}$ components, and deposition of key pollutant species.

Recommended Analyses for Ozone:

- Hourly ozone and maximum 8-hour average (MDA8) ozone values
- Ozone values above certain thresholds (i.e., 60 ppb and other appropriate thresholds)
- Ozone Precursors: NO_X, NO_Y, VOC, speciated VOC, HNO_3, NO, NO_2, PAN, CO, CH_4, SO_2, and NH_3

Recommended Analyses for $PM_{2.5}$:

- Evaluate each $PM_{2.5}$ component separately during high $PM_{2.5}$ episodes
- $PM_{2.5}$ Components: SO_4, NO_3, NH_4, elemental carbon, organic carbon, and crustal elements
- Consider Ammonia (NH_3) data from available AMON sites

Recommended Analyses for SO_4, NO_3, and NH_4 Deposition:

- Weekly results compared to data for NADP wet and CASTNet dry deposition
- Weekly and seasonal averages at individual monitor sites for wet deposition

Assessment of PGM Platform

Diagnostic Evaluation:

- Sensitivity Tests: Different boundary conditions, emissions inputs, or meteorological inputs based on issues identified during the other portions of the platform evaluation.

Analysis Approaches:

- **Plots of Indicator Ratios**: Ratios of species can be useful for assessing if model accurately represents relative emissions rates of precursors and different chemical regimes of ozone sensitivity to VOC and NOx.
  - Example: Model may be biased in simulating absolute concentrations of VOC and NOx due to errors in dispersion but may accurately represent the ratio VOC/NOx.

- **Process Analysis:** Provides diagnostic information on chemical reactions and physical processes that determine species concentrations. Processes include:
  - Net change from Chemistry, Emissions, Deposition, Advection, Diffusion, Vertical Mixing, and chemical production and loss rates from individual reactions.
  - Example: Compare modeled ozone concentrations, output rates of ozone, daily total odd oxygen production rates, and net ozone production in NOx limited and oxidant limited chemical regimes.

Evaluation for Individual Sites & Episodes

Focus on or partition results into subsets:

- **Averaging Period**: Hourly averages and averages that correspond with form of air quality standard or metric being evaluated for each pollutant.

- **Episode Selection**: Limit number of days used in detailed analyses, and assists in providing more intensive evaluation on days most relevant to NAAQS. Episodes could include:
  - **High ambient and modeled concentrations:** For ozone, days when ambient concentrations are greater than 60 ppb.
  - **Days not associated with abnormal conditions:** Model often performs poorly for unusual events, such as stratospheric intrusions, wildfires or dust storms.
  - **Partition days influenced by certain meteorological conditions (cloud cover/precipitation) and surface conditions (snow cover/albedo):** Conditions strongly influence photochemical reactions, formation, and deposition of various pollutants.

Model performance evaluated at individual sites and days ensures:

- Biases do not cancel out;
- Long-term averages reflect model performance on days relevant to NAAQS; and
- Identification of specific periods with good and poor model performance.

Statistical and Graphical Analyses

Recommended Statistical Analyses:

- Number of Data Points
- Mean Model / Observations
- Mean Bias / Error
- Fractional Bias / Error
- Correlation Coefficient

Recommended Graphical Displays (Prioritized):

1. **Time-series Plots (Hourly per site):** Identifies particular times and locations with good or poor performance. Also useful to plot model results for multiple grid cells close to the monitor.
2. **Spatial Plots (Hourly/Daily/Monthly):** Identifies times and locations with good or poor performance, and where model accurately simulates observed levels but misplaces the location.
3. **Vertical Profiles:** Determines how well the model represents the atmospheric profiles and boundary layer heights.
4. **Scatter Plots (Hourly):** Assesses model performance for a range of levels.
5. **Bugle Plots:** Assesses model performance as concentrations increase/decrease in magnitude.
6. **Q-Q and Box-Whisker Plots:** Assesses the dynamic range of the model.

Reporting MPE Results

Goal:

- Summarize degree of confidence in model platform as a tool to inform planning process, and to determine how reliable model predicts the response of ozone, $PM_{2.5}$ and deposition to emissions changes.
- Compilation of all analyses into comprehensive report that describes strengths and weaknesses and how model platform should be used in light of evaluation findings.

Reports:

- For each component of PGM platform, generate a stand-alone report that summarizes:
  - Summary of datasets (monitor locations and density) and model input and configuration.
  - Sample graphical displays that characterize individual pollutants by various source categories across the model domain.
  - Summary of sensitivity tests that investigated poor model performance.
  - Comparison to evaluations completed in other similar studies.
  - Discussion of the strengths and weaknesses indicated by evaluation for various parameters, time periods, and locations.
  - Outline lessons-learned and model limitations/uncertainties that may require further model development, improvement, and/or diagnostic evaluation.
- Overall Memo: High-level memo outlining how the model platform should be used in light of evaluation findings.

Progression of IWDW – WAQS MPE Efforts

Model Platform	2008 (36/12/4 km)	2011 (36/12/4 km)
AQ PGM Platform (Focus)	CAMx: 12 km	**CAMx and CMAQ: 4 km**
IC/BC Evaluation	No	**Yes**
Emissions/Meteorology/PGM Evaluation	Yes	Yes
Pollutants Evaluated	O3, NOx, Speciated PM, AQRVs	O3, NOx, **Speciated VOCs** and PM, CH4, NH3, AQRVs
Results Averaging Approach	Hourly, Monthly, Seasonal Average Across; Domain, Network, State	Hourly, Monthly, Seasonal, Diurnal Average Across; Domain, Network, State, **Individual Sites**
Statistical Evaluation	Yes	Yes
Diagnostic Evaluation	No	**BC (GEOS-Chem vs MOZART), WRF Winter Configuration, Emissions Adjustments**
Dynamic Evaluation	No	Yes (Limited: 2008 and 2011)
Report	Protocols, PGM MPE Report	**Protocols, Emissions (2011 and 2008 comparisons), WRF, PGM**
Distribution/Review of Results	Upon Request/Summarized in Report	**Online Access**/Summarized in Report

OVERVIEW: IWDW Visualization Tools

Monitor Data

Visibility Summary
View line and bar charts of deciview trends and aerosol haze budgets on the clearest and haziest days based on data from the IMPROVE Aerosol monitoring network.

Ozone Summary
View line and bar charts of the 4th Highest 8-Hour Daily Ozone Average, the W126 Exposure Index, and the SUM06 Exposure Index based on data from the EPA's Air Quality System (AQS).

Wet Deposition Summary
View line and bar charts of wet nitrate, wet ammonium, and wet sulfate trends and composition based on data from the National Atmospheric Deposition Program (NADP).

Dry Deposition Summary
View line and bar charts of dry nitric acid, ammonium, nitrate, and sulfate trends and composition based on data from the EPA's Clean Air Status and Trends Network (CASTNet).

Emissions Data

Emissions Review Tool
View charts and graphs of annual emissions totals for States, Counties, and Source Classification Codes (SCCs) from several different 3SAQS modeling scenarios.

Emissions Review Map
View spatial display of annual emissions totals for States, Counties, and Source Classification Codes (SCCs) from several different WAQS modeling scenarios.

Modeling Data

Model Performance Evaluation Plots
View a wide variety of scatter plots, soccer plots, bar charts, and maps demonstrating model performance for several modeling scenarios in the Three-State Air Quality Study (3SAQS).

Model-To-Observation Comparison Tool
View network-wide and site-specific time series charts of modeled and observed parameters from several different air quality monitoring networks in the Intermountain West region.

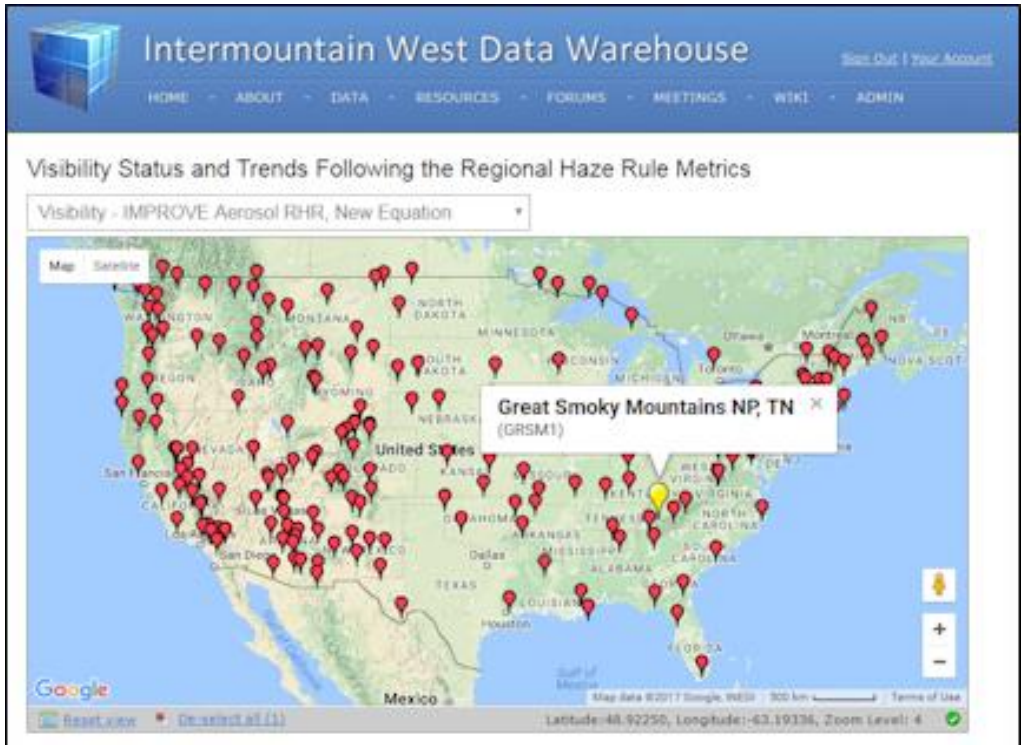
Source Apportionment Visualization Tools and Resources
Links to Visualization Tools for 2008b, 2011a and 2011b based Source Apportionment tools; Source Apportionment data download and documentation.

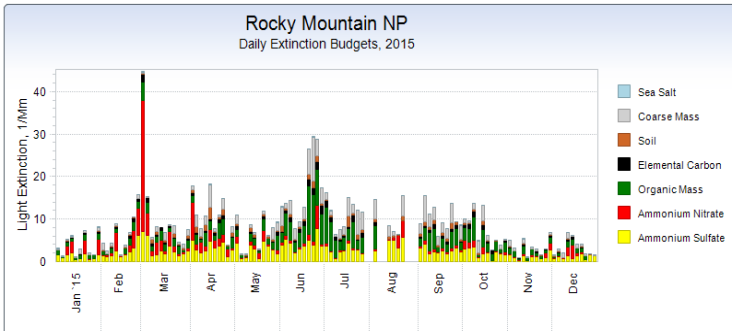
Visualization Tools: Monitoring Data

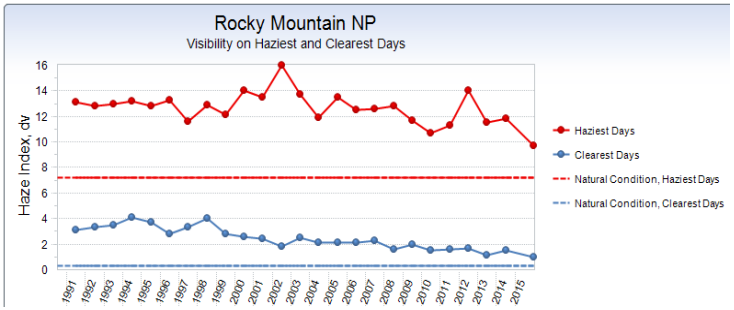
Purpose:
Present visual summaries of monitoring data using AQS, CASTNET, IMPROVE networks.

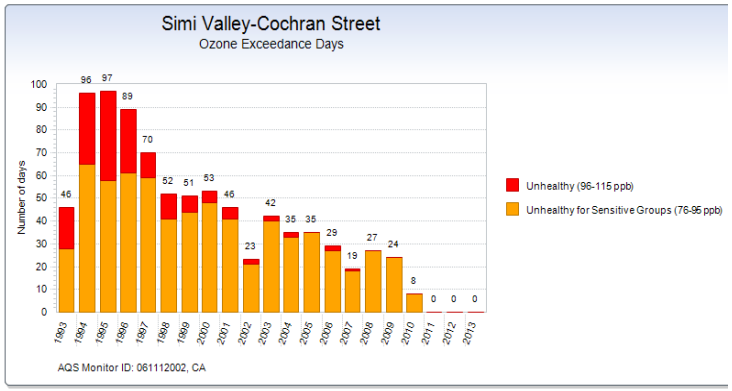
Features:

- Data aggregation and analysis
- Map-based selection of monitoring sites
- High-level interpretations of the data







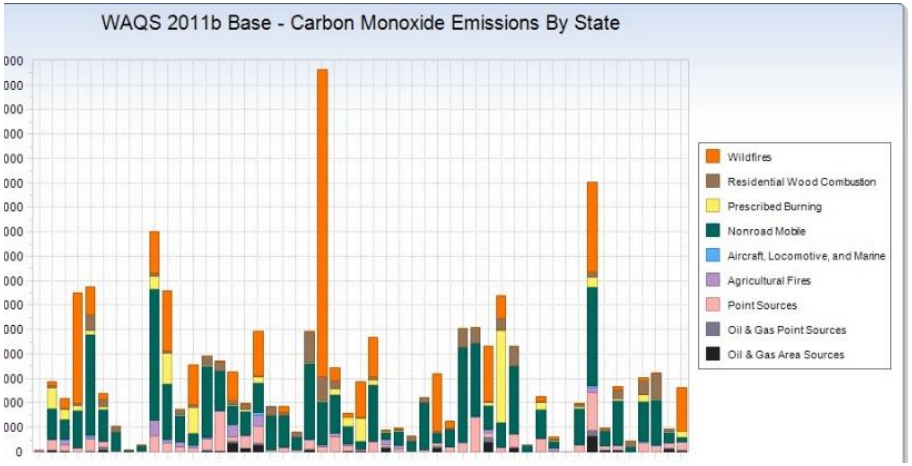


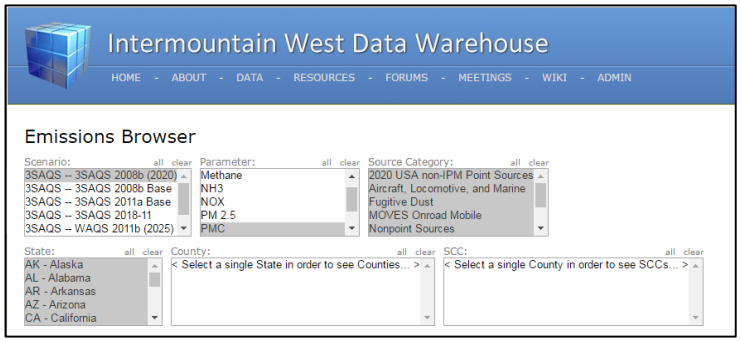
Visualization Tools: Emissions

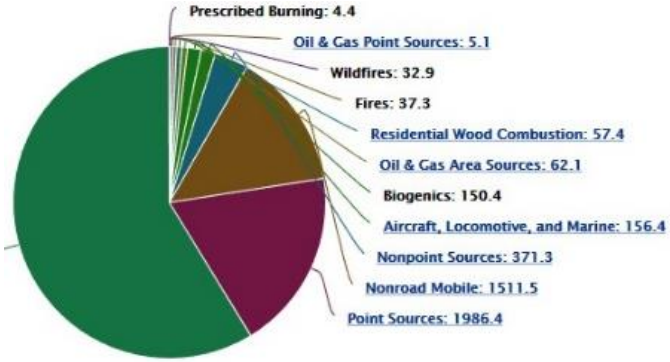
Purpose:
Breakdown of emissions by state, county, & source category for Base and Future years.

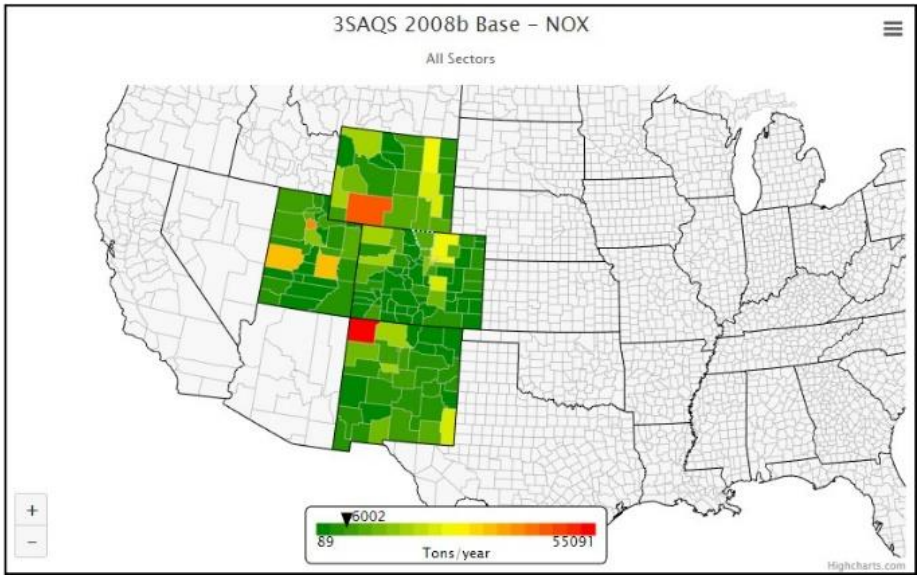
Features:

- Pie and bar charts and maps of emissions for specified parameter, source categories, and SCC codes at state or county levels
- Chart data downloadable







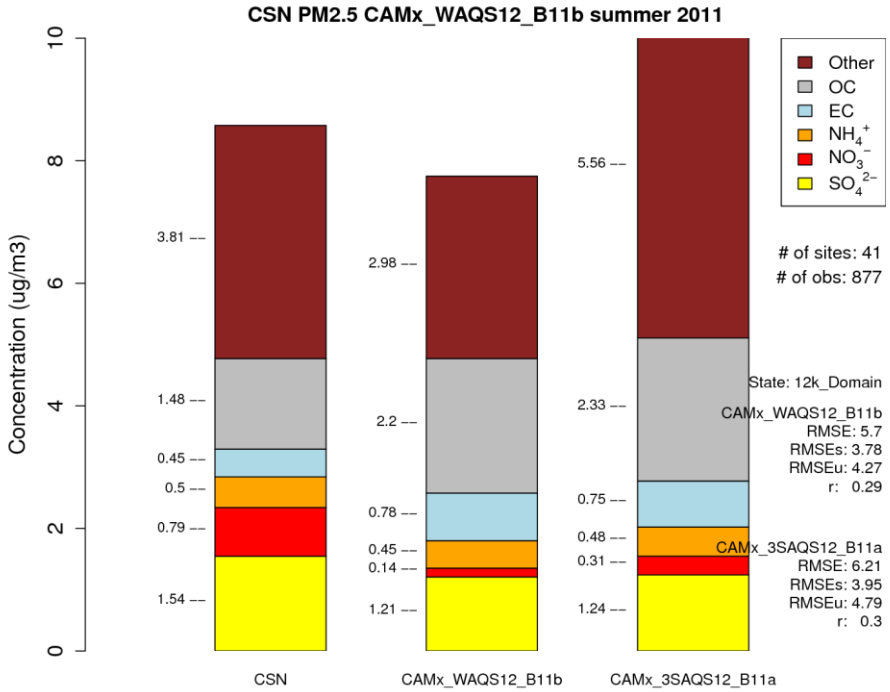


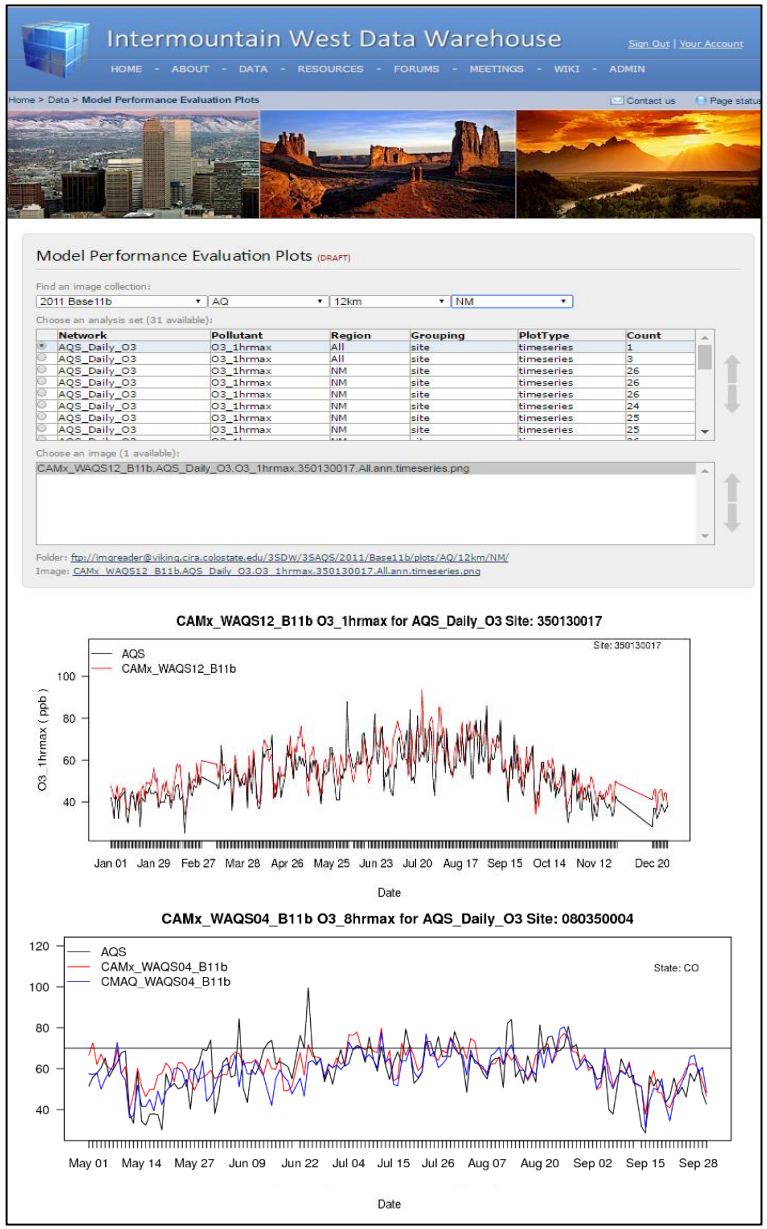
Visualization Tools: PGM MPE

Purpose:
Provide site-specific time-series plots of modeled and observed parameters leveraging PAVE and AMET.

Features:

- Chart data visible in browser
- Mouse over to get specific values
- Displays and images downloadable
- Image directories open for browsing



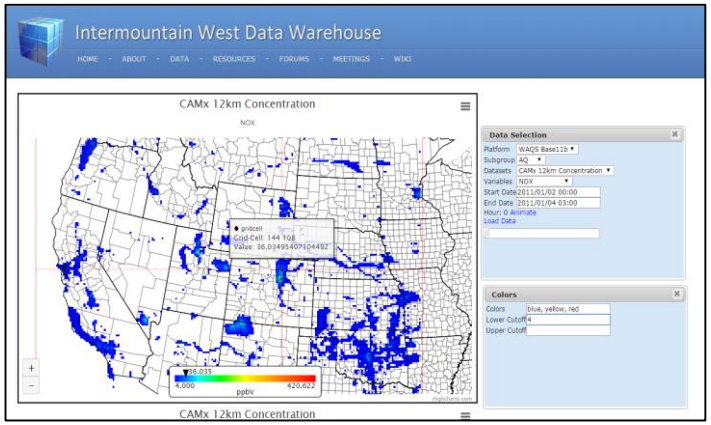


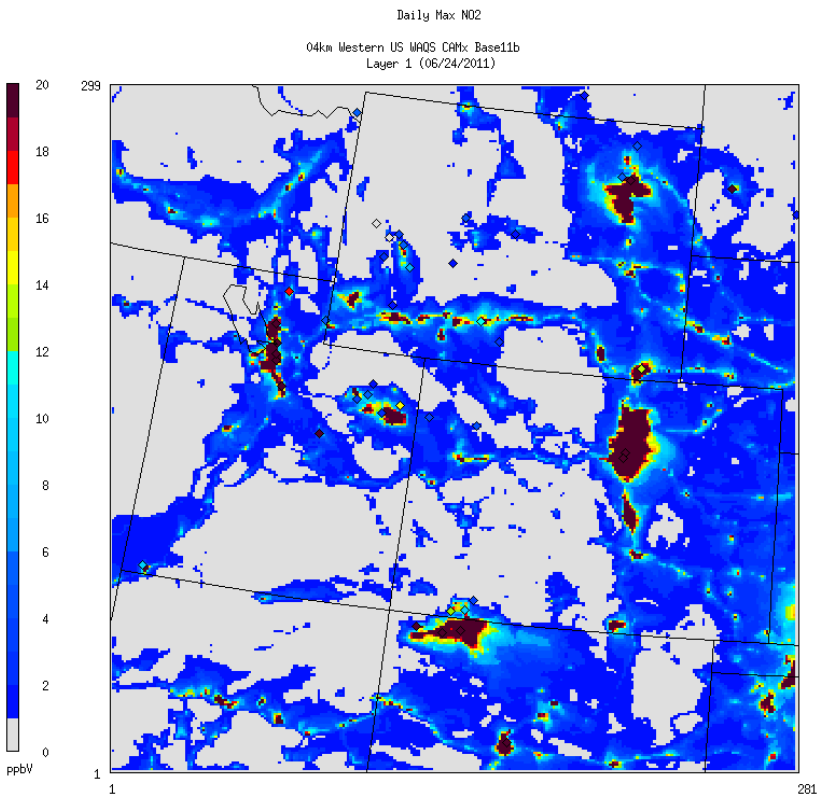
Visualization Tools: PGM MPE

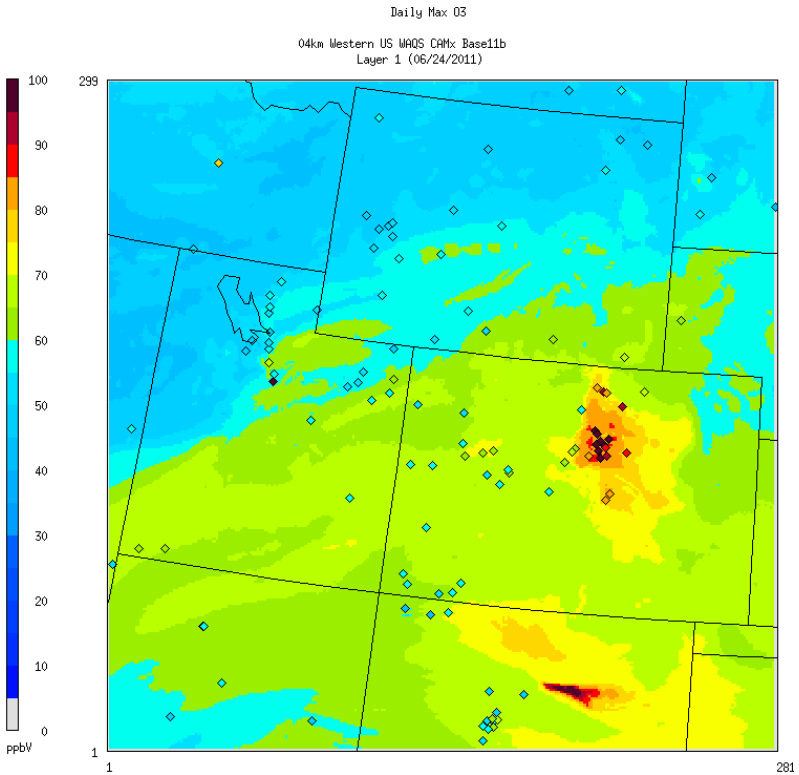
Purpose:
Provide interactive display of gridded data and grid cell time series.

Features:

- Rendering performed in browser
- User specified coloring
- All configuration embedded in URL for quick reference







Benefits and Next Steps/Future Needs

Benefits of MPE Checklist to WAQS:

- Streamlines approach for conducting model evaluations
- Comprehensive performance evaluation to inform users of model issues and applicability to various projects
- Identifies potential resources (funding and computing needs) for completing evaluations that are relevant to western U.S.
- Outlines approach for documenting model performance and gaps for transparency and development of future platforms

IWDW-WAQS Next Steps/Future Needs:

- **2014 PGM Platform:** Developing and anticipated release will be early 2019
- Continue development of model post-processing capabilities and tools
- Wish List – Leveraging of Resources and Tools:
  - In-house MPE plot browser that displays plots of model-to-obs and model-to-model comparisons generated using AMET
  - Vertical profile visualization tools
  - Tools that allow for real-time analysis
  - Coordinate with other group to leverage tools

Website: http://views.cira.colostate.edu/tsdw/