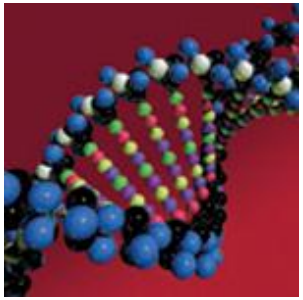
WestJumpAQMS Progress Report – 2008 Base Case and Preliminary Source Apportionment Modeling



ENVIRON International Corporation
Alpine Geophysics, LLC
UNC Institute for the Environment

June 20, 2013

WESTERN REGIONAL AIR PARTNERSHIP

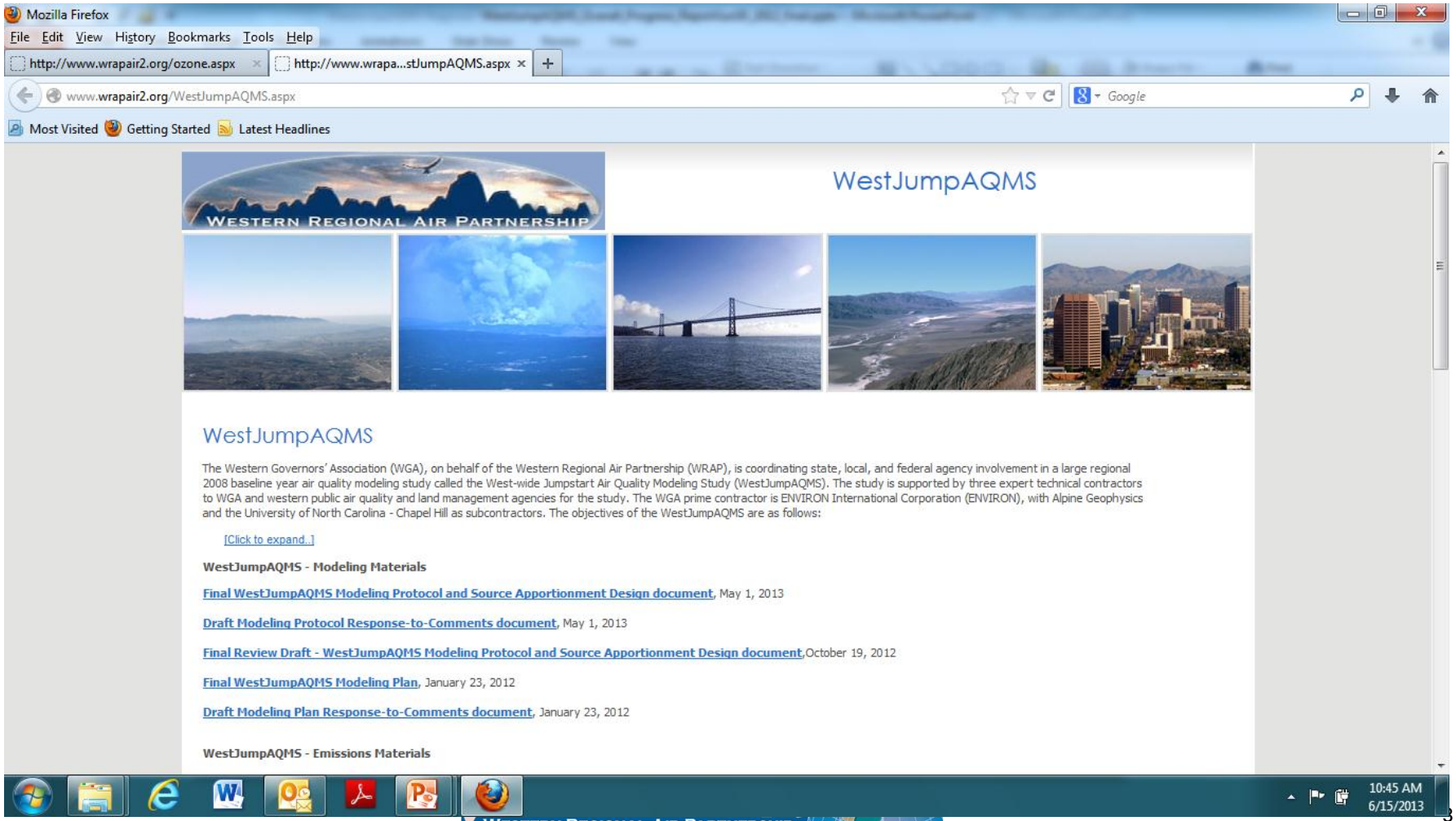
ENVIRON

Background

- Future Ozone standards could result in many areas in western U.S. being nonattainment
- Western Regional Air Partnership (WRAP) has initiated the West-wide Jump Start Air Quality Modeling Study (WestJumpAQMS) to:
  - Initiate next generation of regional technical analysis for ozone planning in the western U.S.
  - Continue work conducted at the WRAP Regional Modeling Center (RMC) and leverage recent air modeling studies
  - Provide a preliminary assessment of the role of ozone transport to elevated ozone concentrations across the West

Background

- Contracting team of ENVIRON, Alpine Geophysics and UNC IE
- WestJumpAQMS Website with products to date



WRAP RMC vs. WestJumpAQMS

Parameter	WRAP RMC	WestJump AQMS
Modeling Year	2002	2008
Met Model	MM5	WRF
36 km CONUS	165 x 129	165 x 129
12 km WESTUS	Not Used	235 x 240
4 km IMWD	NA	325 x 525
Vertical	34	37
Total Grids	723,690	9,187,470 (13x grids) (81x resolution)
AQ Model	CMAQ	CAMx & CMAQ
36 km	148 x 112	148 x112
12 km	NA	227 x 230
4 km	NA	164 x 218
Layers	19	25
Total Grids	314,944	2,,613,450 (8x grids)

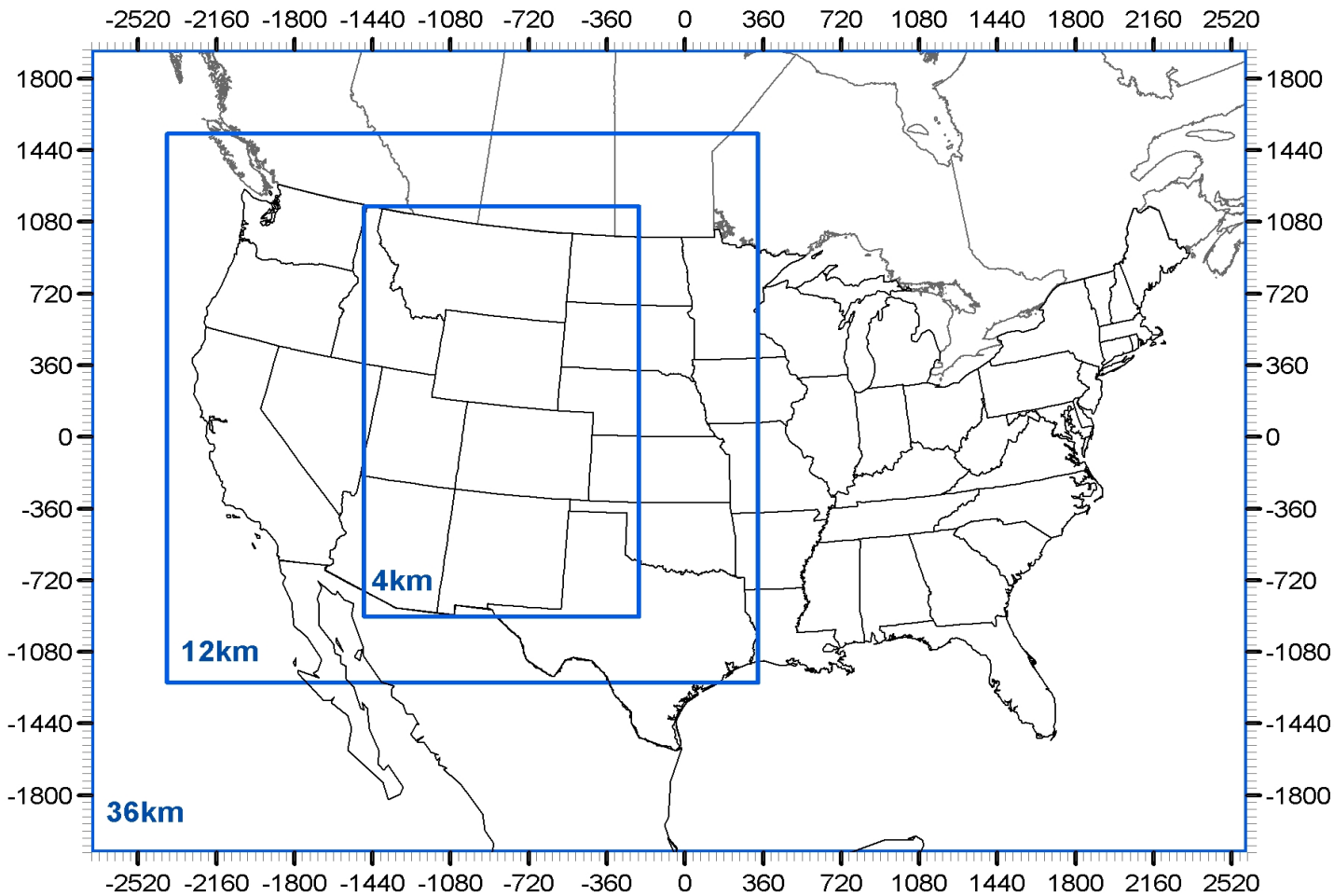
WestJumpAQMS Completed Tasks (today's topic)

- WRF Application/Evaluation
- 2008 Oil and Gas Emissions Update
- 16 Emissions Summary Memorandums
- SMOKE Emissions Modeling
- CAMx Model Input Development
- Calculate Basin-wide WRAP Phase III O&G EFs for use in 2011 NEI
- **CAMx 2008 36/12 km Base Case**
  - **Model Performance Evaluation**
- **CAMx 2008 State-Specific Ozone Source Apportionment Modeling**

WestJumpAQMS Ongoing Tasks

- CAMx 2008 State-Specific PM Source Apportionment Modeling
- CAMx 2008 Source-Category-Specific Ozone and PM Source Apportionment Modeling
- CMAQ 2008 Base Case Modeling
- CAMx 4 km Impact Assessment Domain (IAD) Inputs
- MOZART vs. GEOS-Chem Boundary Condition Sensitivity
- Data Transfer to Three State Data Warehouse (3SDW)
- Final Report and Two more Webinars
  - July 17 @ 10am MDT: 4 km IAD; Outline Final Report; State-specific PM source apportionment; MOZART vs. GEOS-Chem BC sensitivity
  - Mid-August: Source category-specific ozone and PM source apportionment; final report; wrap up

36 km CONUS; 12 km WESTUS & 4 km IMWD processing domain



Modeling Domain

Summary of CAMx 2008 36/12 km Inputs

- WRF 2008 36/12 km Meteorology
- MOZART Global Model Boundary Conditions
- 2008 Base Case Emissions
  - WRAP Phase III 2008 Oil and Gas Emissions
    - 2008 NEI O&G outside of WRAP Basins
  - MEGAN Biogenic Emissions
  - Hourly CEM for Electrical Generating Units (EGUs)
  - 2008 National Emissions Inventory (NEIv2)
  - Fire INventory from NCAR (FINN) [Base08a&b]
  - DEASCO3 Fire Emissions (Base08c)

CAMx 2008 36/12 km Base Cases

- Base08a – FINN Fires -- May, Jun and Jul 2008
- Base08b – FINN Fires – 2008 36/12 km Annual
  - Correct double counting of SUIT O&G emissions (Southwest CO) from WRAP and 2008 NEI
- Base08c – DEASCO3 Fires (WF, Rx & Ag) – 2008 36/12 km Annual
  - Correct O&G county swapping
  - Model performance evaluation
    - ozone, $PM_{2.5}$ and speciated $PM_{2.5}$ (SO4, NO3, NH4, EC, OA, Soil and OPM2.5)
    - 36 km CONUS and 12 km WESTUS domains and by western state

CAMx 2008 36/12/ km Base08c Ozone MPE

- Ozone Model Performance Goals
  - Bias ≤ ±15% and Error ≤ 35%
  - Original EPA (1991) guidance used Mean Normalized Bias (MNB) and Gross Error (MNGE)

$$\frac{1}{N}\sum_{i=1}^{N}\frac{(P_i - O_i)}{O_i}$$

  - Simon, Baker and Philips (2012):
    - Don't recommend MNB as not balanced and can blow up at low observed concentrations so recommend:
  - Fractional Bias (FB):

$$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$$

    - Bounded (≤±200%)
  - Normalized Mean Bias (NMB):

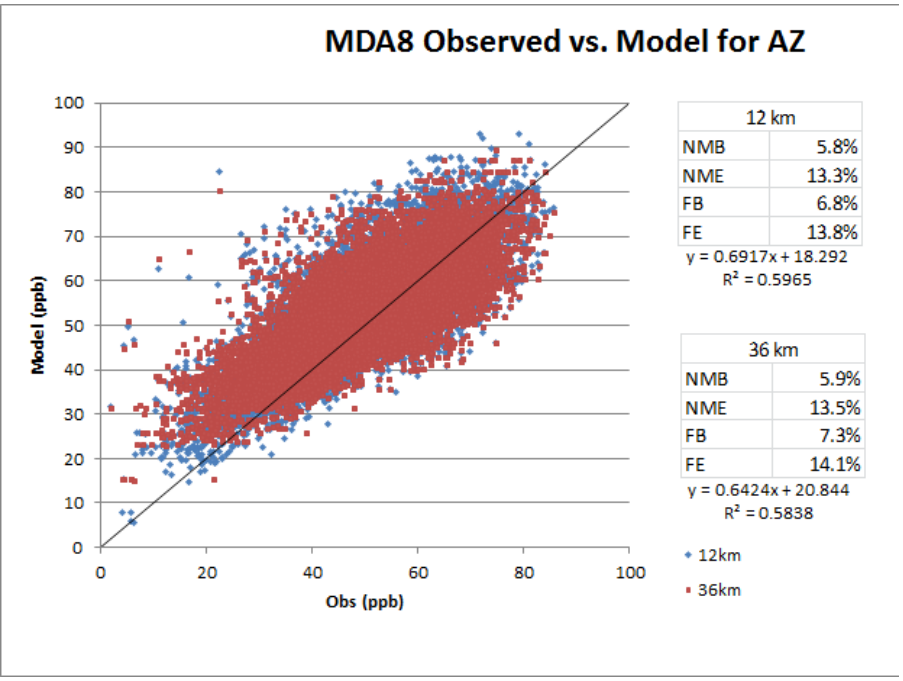
$$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N}O_i}$$

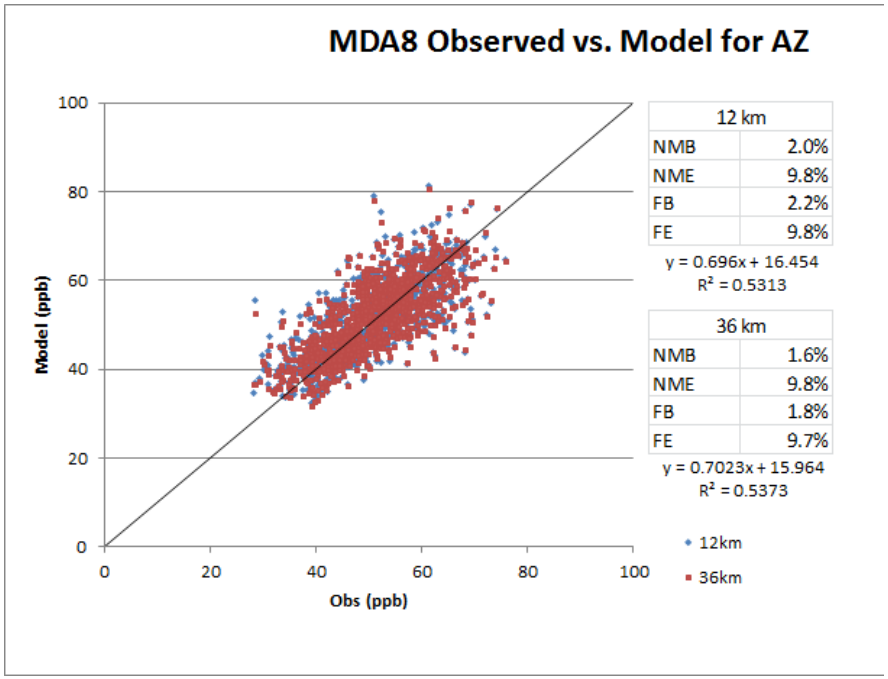
Ozone Model Performance

- Daily Maximum 8-Hour Ozone (DMAX8)
- Matched by day and location (grid cell)
- Scatter Plots of Predicted and Observed DMAX8 with Model Performance Statistics:
  - Fractional Bias (FB) and Error (FE)
  - Normalized Mean Bias (NMB) and Error (NME)
  - Correlation Coefficient (R^2)
  - Regression Equation
- By western state for:
  - AQS monitors (urban oriented)
  - CASTNet monitors (rural focused)

Arizona 36 km (red) and 12 km (blue) DMAX8

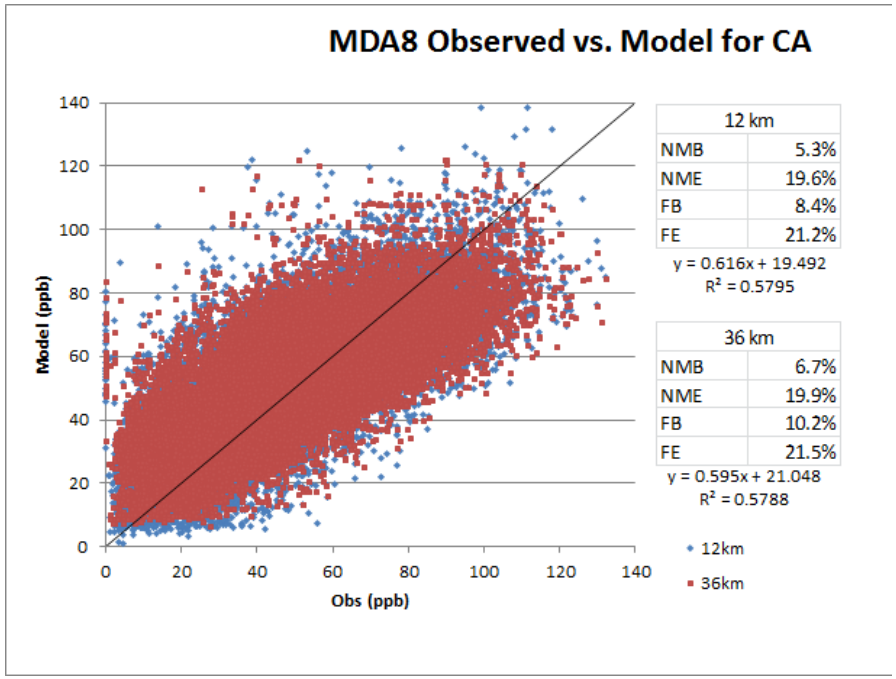
- AQS Monitors
  - NMB = 6% & FB = 7%
  - NME = 13% & FE = 14%
- CASTNet Monitors
  - NMB = 2% & FB = 2%
  - NME = 10% & FE = 10%

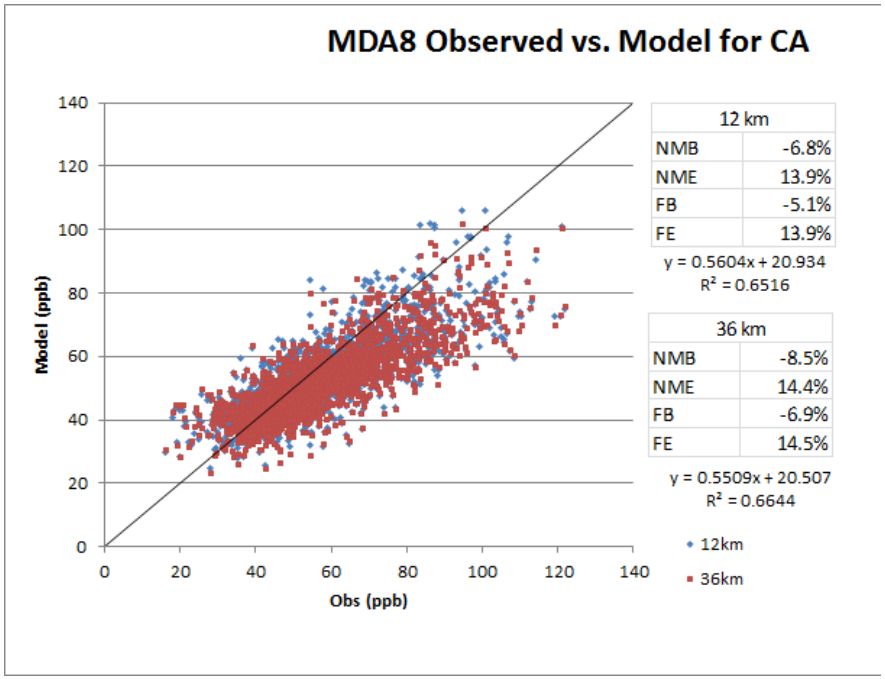




California 36 km (red) and 12 km (blue) DMAX8

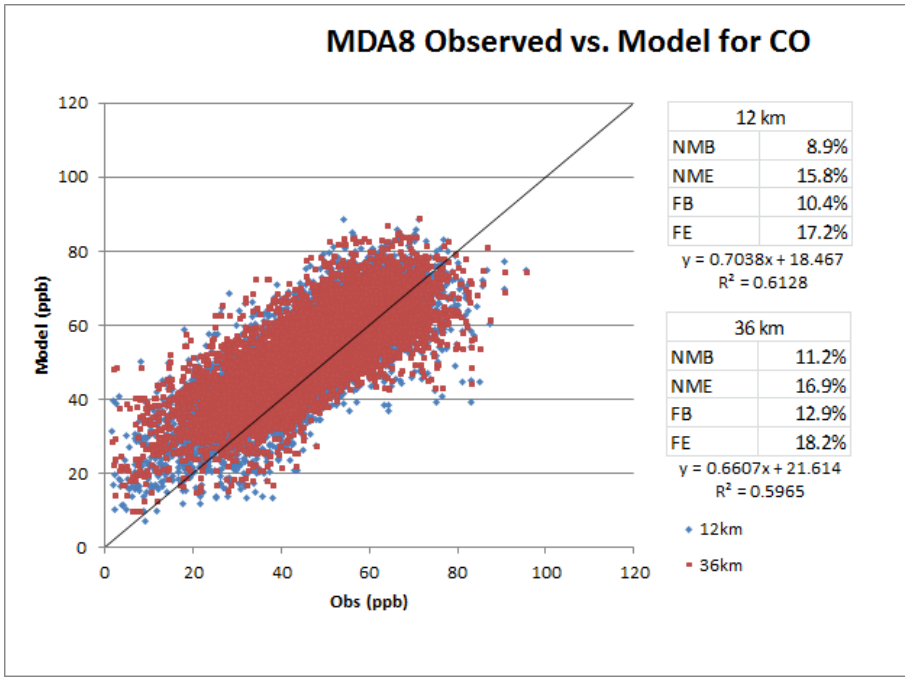
- **AQS Monitors**
  - NMB = 5% & FB = 8%
  - NME = 20% & FE = 21%
- **CASTNet Monitors**
  - NMB = -7% & FB = -5%
  - NME = 14% & FE = 14%

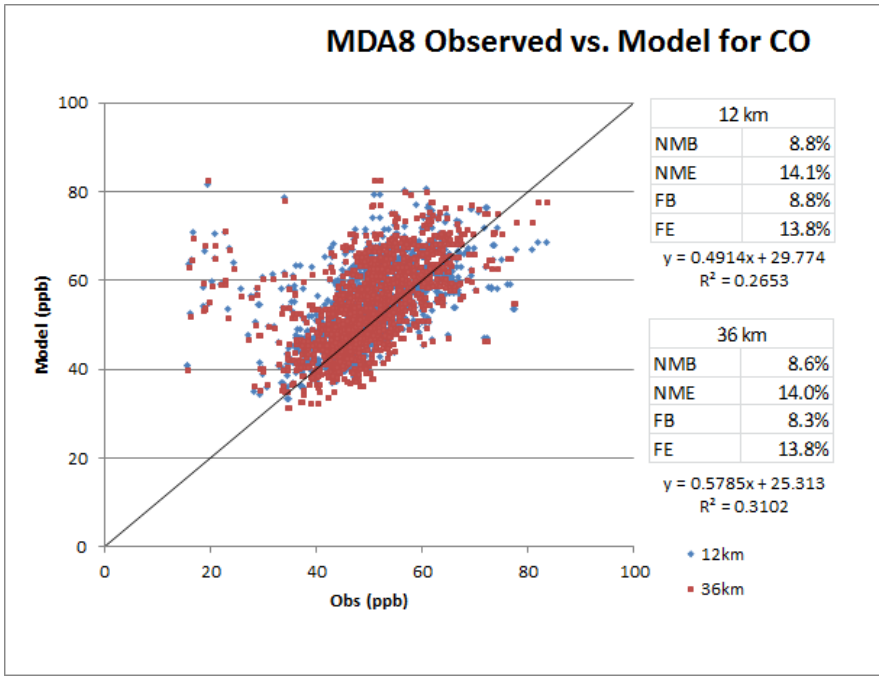




Colorado 36 km (red) and 12 km (blue) DMAX8

- **AQS Monitors**
  - NMB = 9% & FB = 10%
  - NME = 16% & FE = 17%
- **CASTNet Monitors**
  - NMB = 9% & FB = 9%
  - NME = 14% & FE = 14%

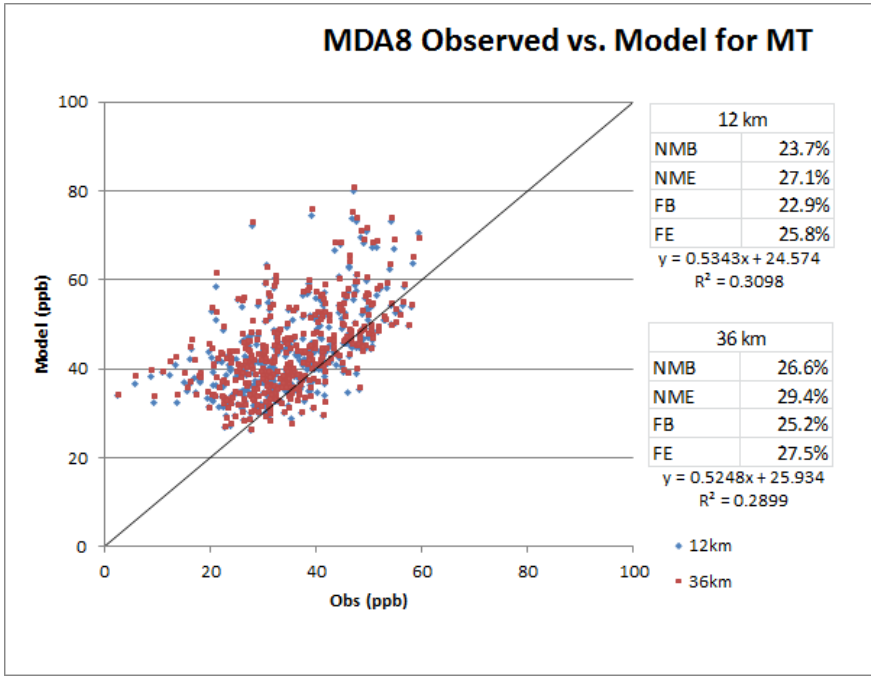


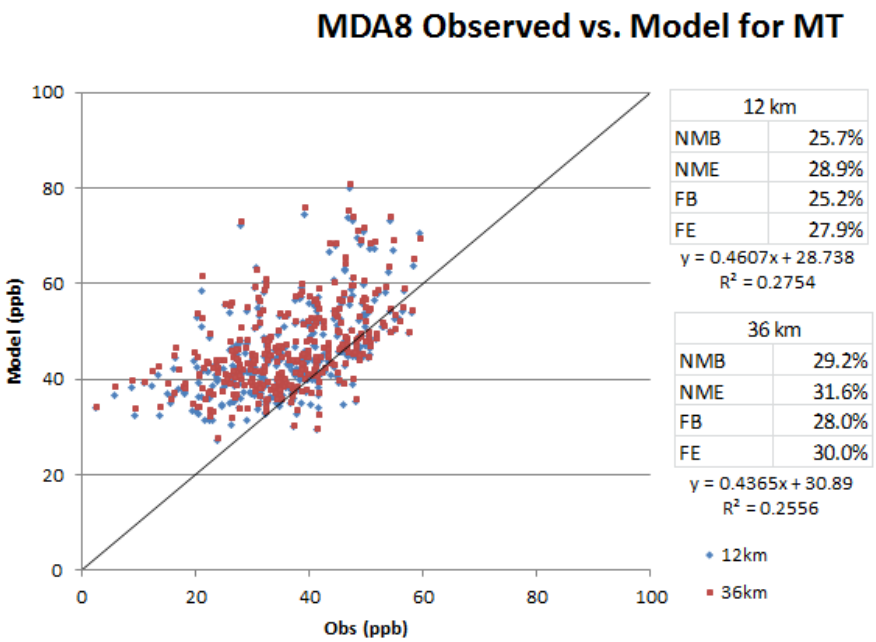


CASTNet DMAX8 overestimations due to modeled stratospheric ozone intrusions when none occurred [Apr 11 (102), May 8 (129) and Jun 13 (165) – (JDay)]

Montana 36 km (red) and 12 km (blue) DMAX8

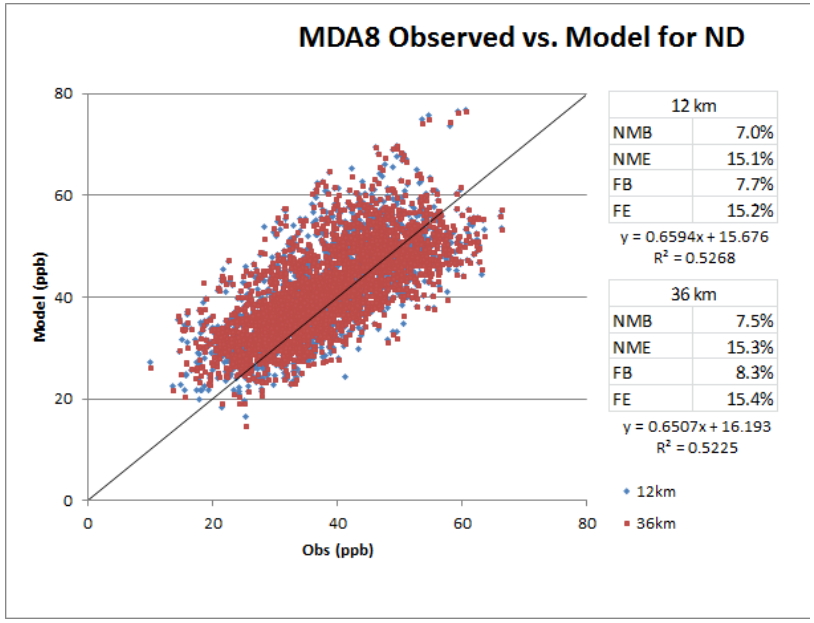
- **AQS Monitors**
  - NMB = 24% & FB = 23%
  - NME = 27% & FE = 26%
- **CASTNet Monitors**
  - NMB = 26% & FB = 25%
  - NME = 29% & FE = 28%

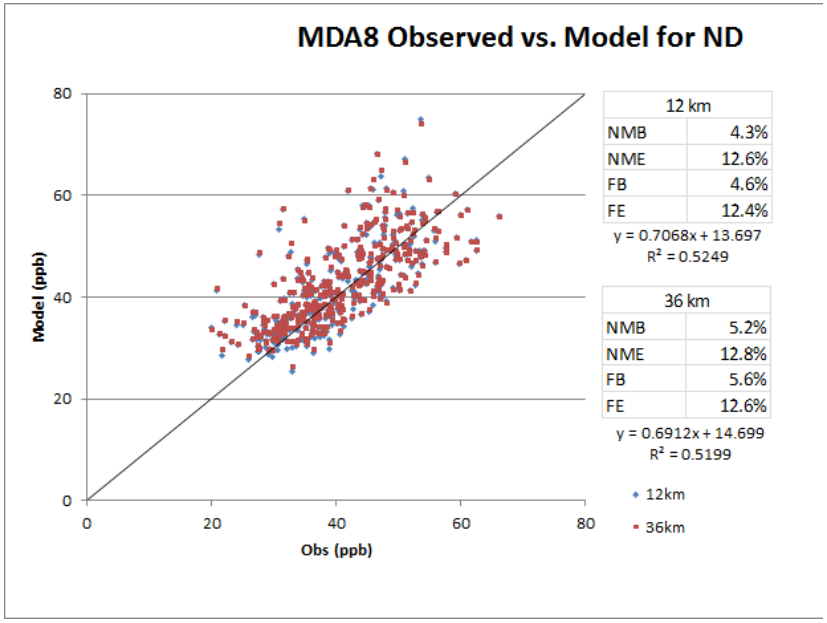


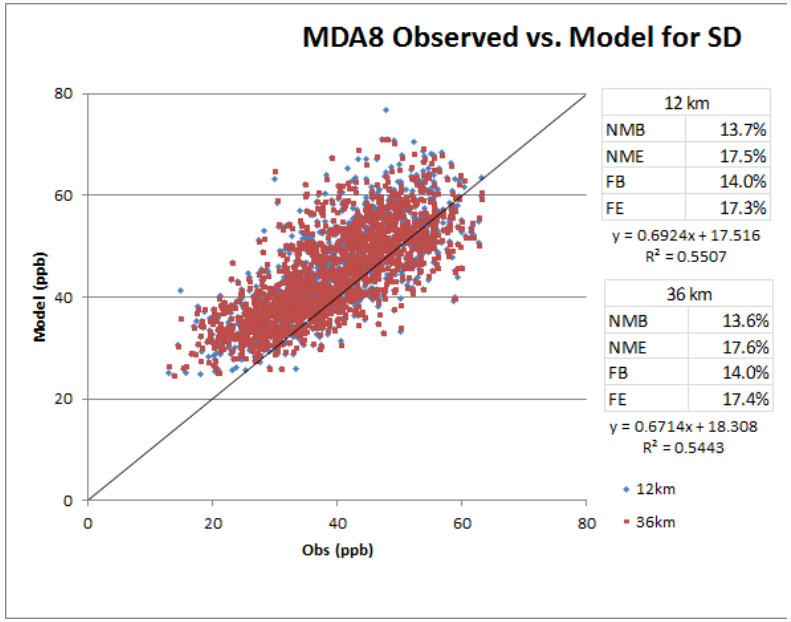


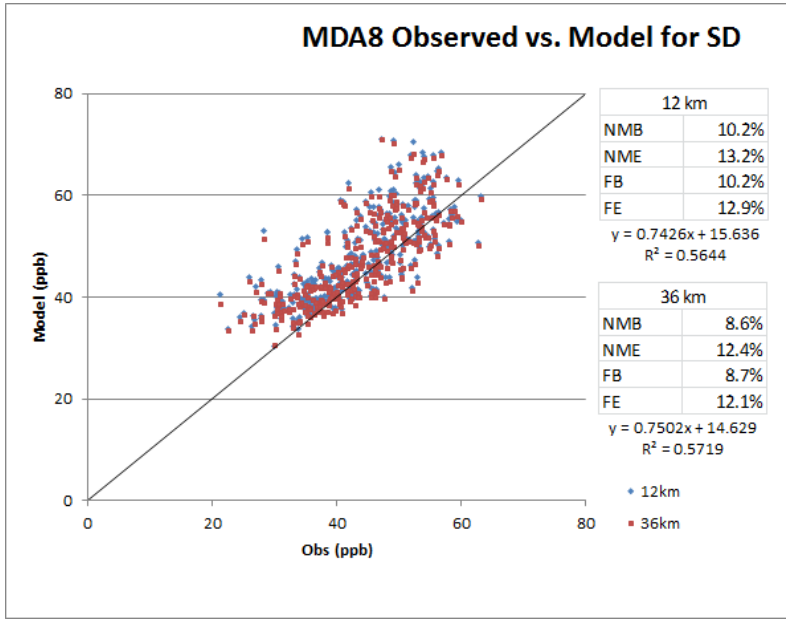
Cause for overestimation under investigation [CASTNet consists of one site, Glacier]

ND and SD 36 km (red) and 12 km (blue) DMAX8

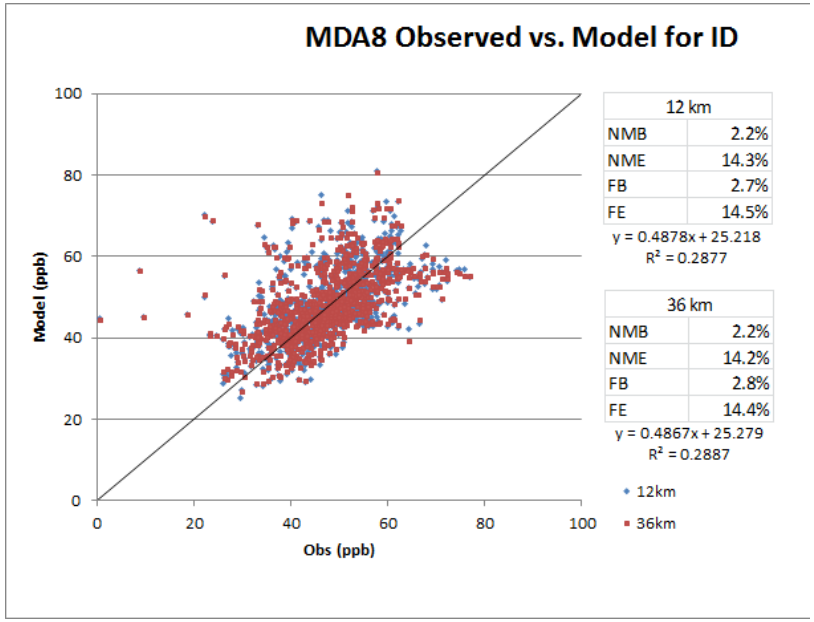




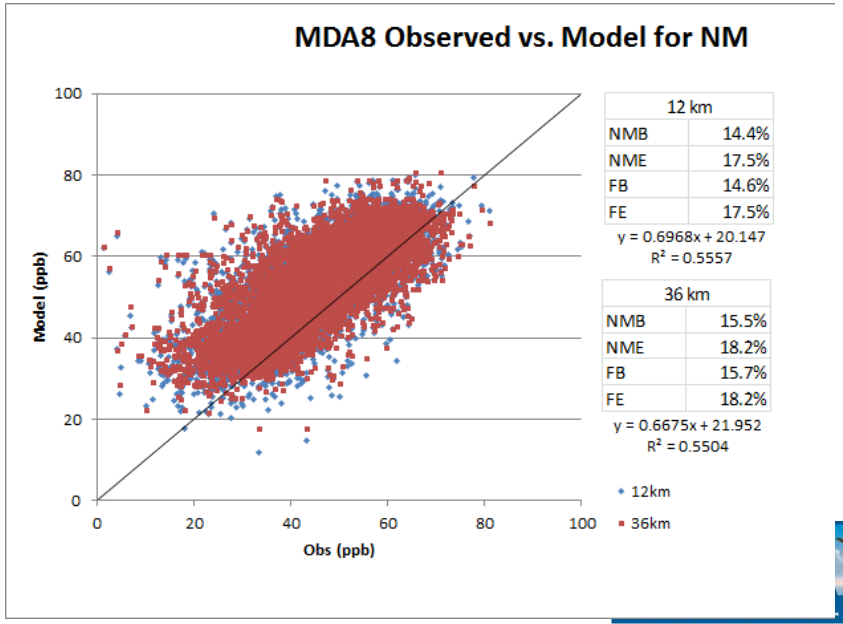


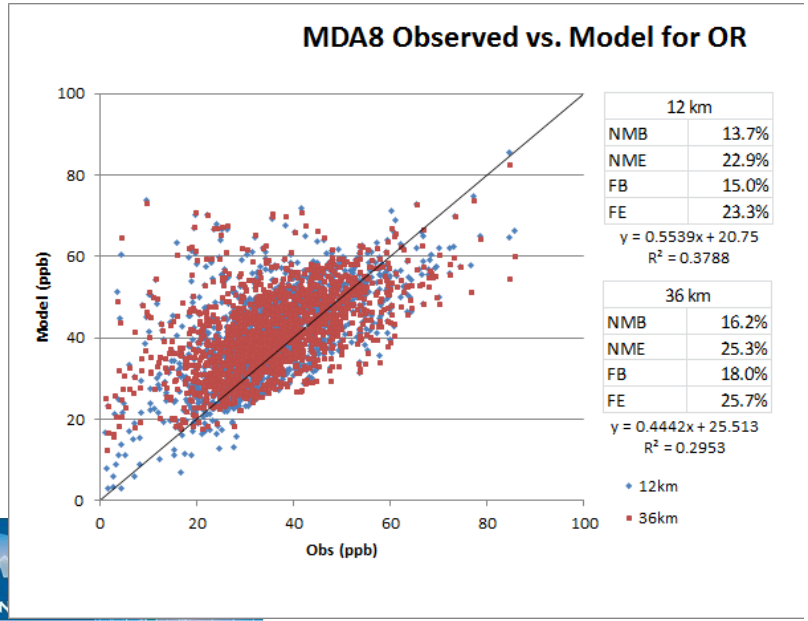


ID, NM and OR DMAX8 -- AQS Only



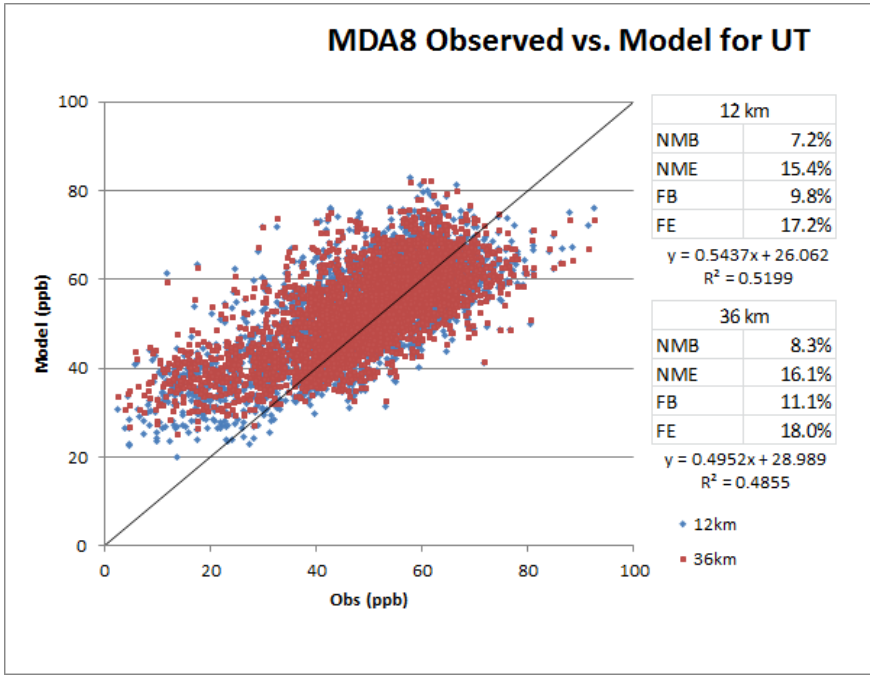
- Idaho low bias (2-3%)
- NM and OR overestimation (bias = 14% to 23%)

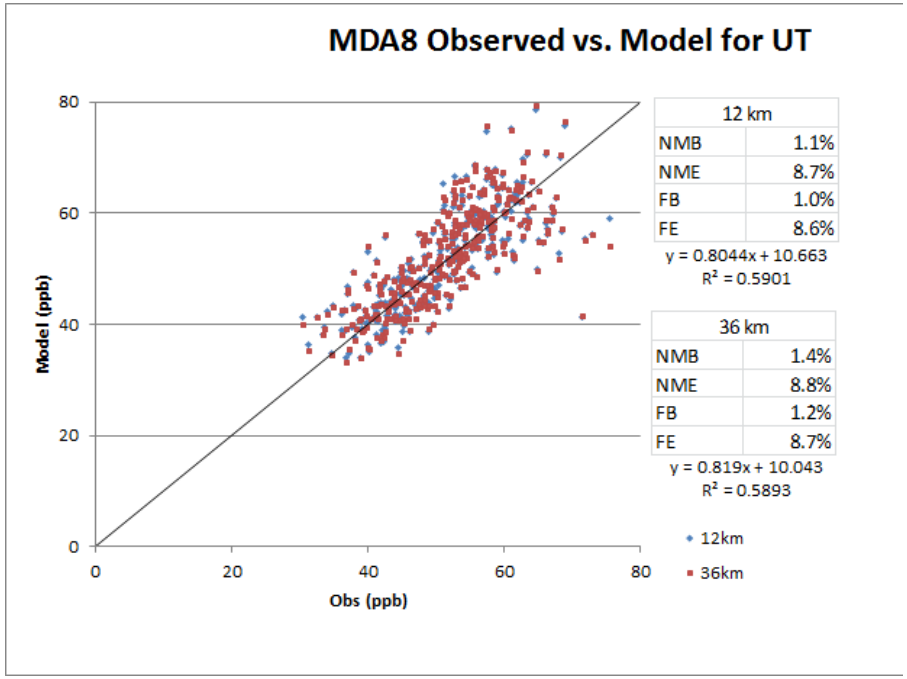




Utah 36 km (red) and 12 km (blue) DMAX8

- **AQS Monitors**
  - NMB = 7% & FB = 10%
  - NME = 15 & FE = 17%
- **CASTNet Monitors**
  - NMB = 1% & FB = 1%
  - NME = 9% & FE = 9%

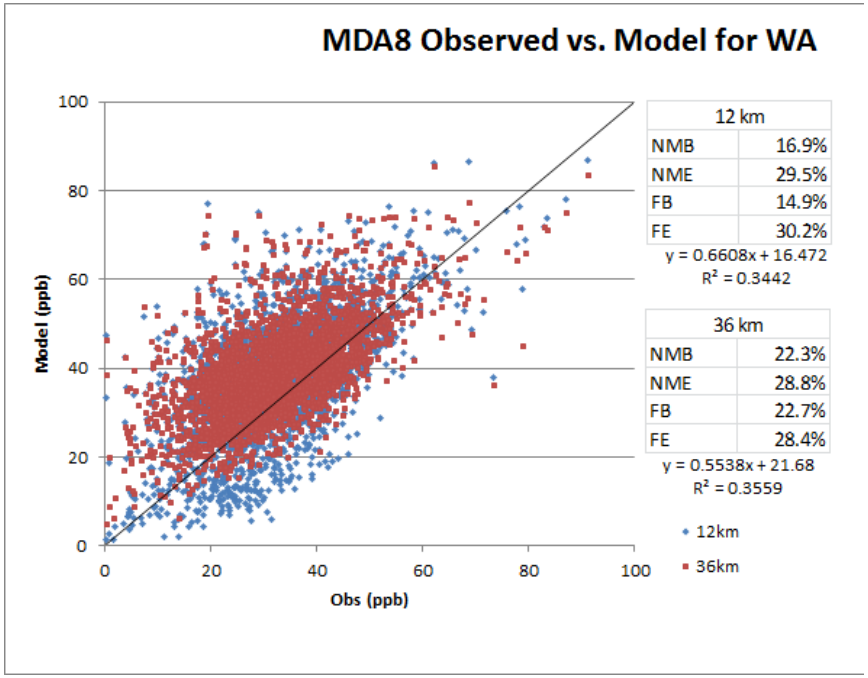


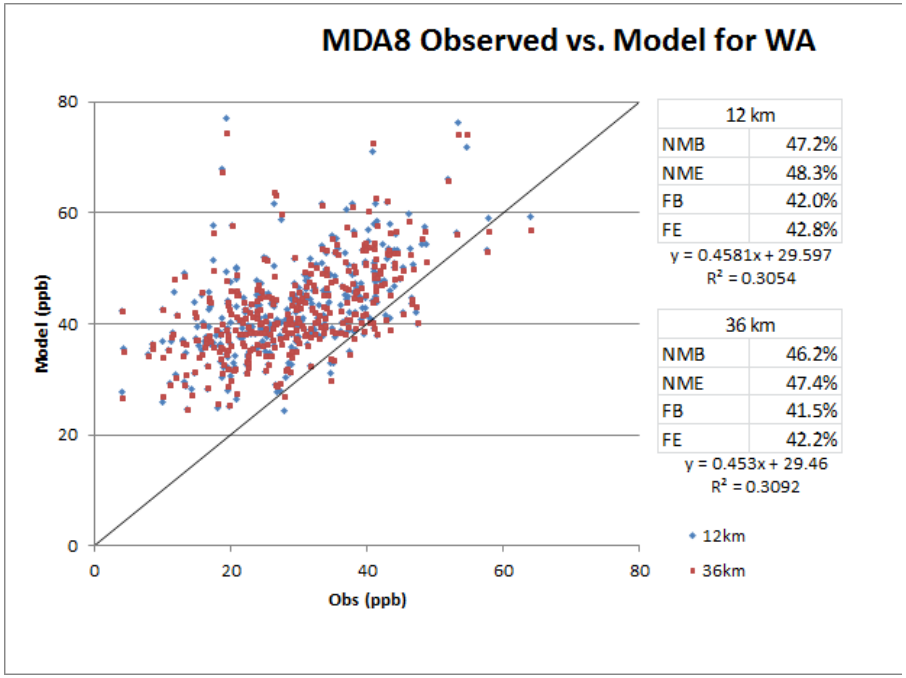


AQS overestimation at low end due to urban monitoring sites and coarse grid.
Very good ozone performance at CASTNet (Canyonlands).

Washington 36 km (red) & 12 km (blue) DMAX8

- **AQS Monitors**
  - NMB = 17% & FB = 15%
  - NME = 30% & FE = 30%
- **CASTNet Monitors**
  - NMB = 47% & FB = 42%
  - NME = 48% & FE = 43%

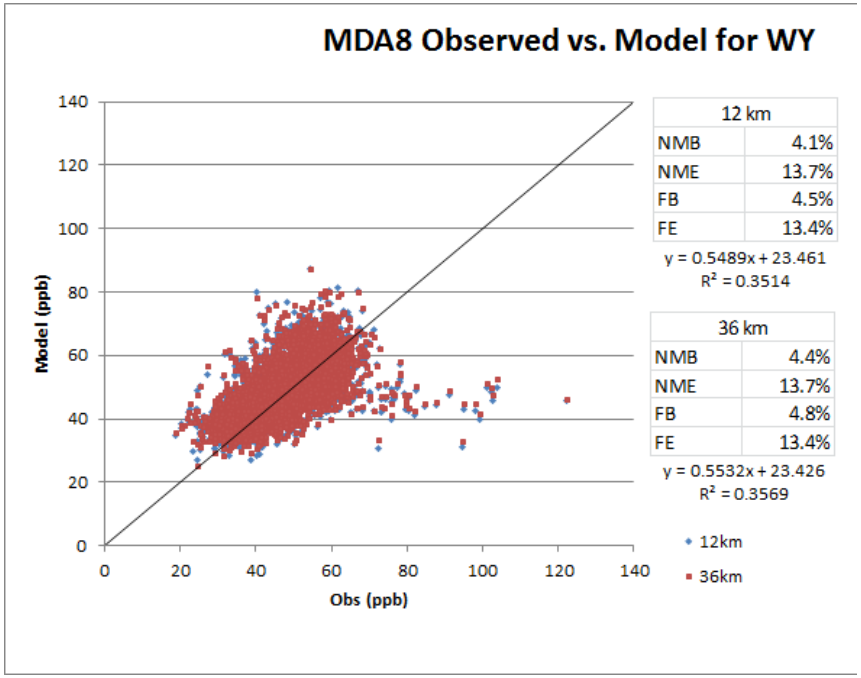


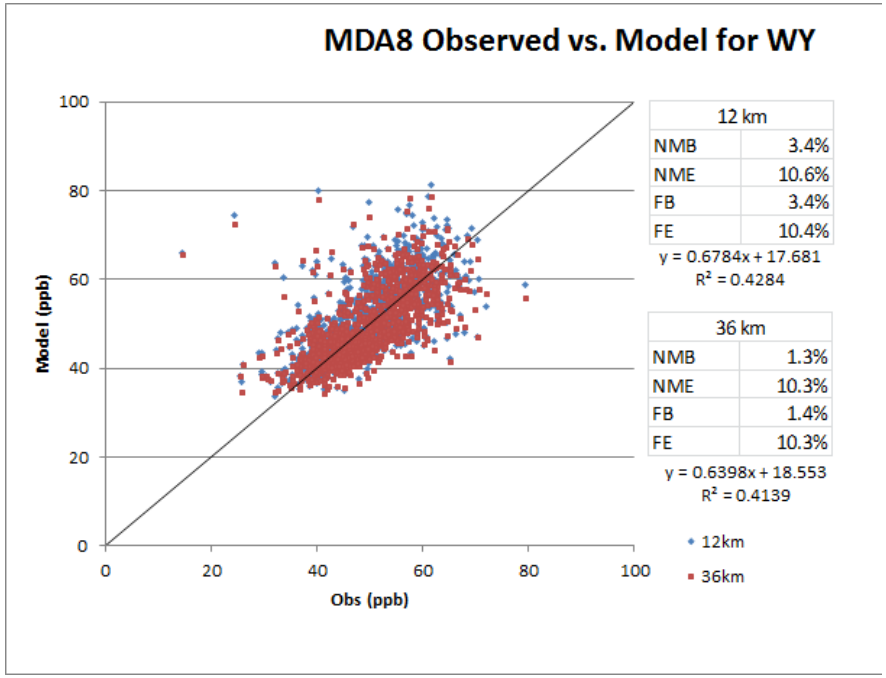


CASTNET (MOR & NCS) has severe overestimation bias partly due to stratospheric intrusion (e.g., highest modeled DMAX8 = 77 ppb at MORA on May 27).

Wyoming 36 km (red) & 12 km (blue) DMAX8

- **AQS Monitors**
  - NMB = 4% & FB = 5%
  - NME = 14% & FE = 13%
- **CASTNet Monitors**
  - NMB = 3% & FB = 3%
  - NME = 11% & FE = 10%





Model not configured to simulate high winter DMAX8 ozone in JPAD (e.g., 122 ppb at Boulder on Feb 21, 2008). CASTNet likely modeled strat ozone in Apr (PND & YEL)

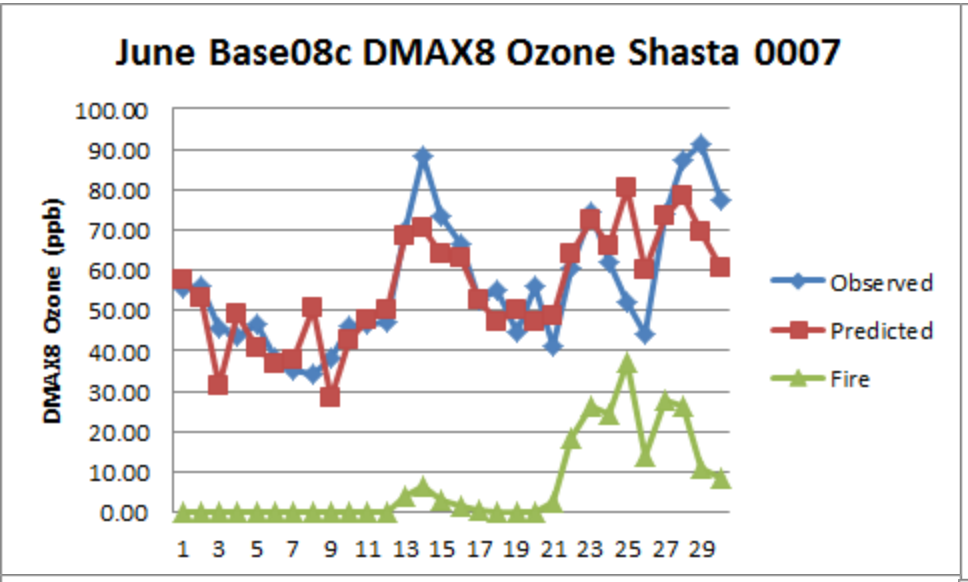
Summary Base08c DMAX8 Ozone Performance

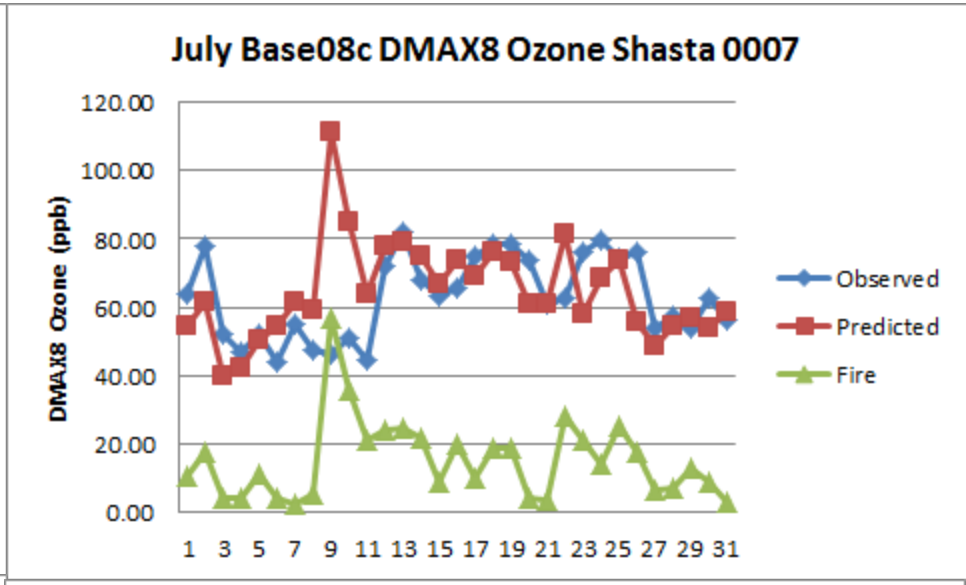
- Mostly reasonable performance with low bias and error (some positive bias tendency)
  - Larger overestimation bias in WA, NM, OR and MT
  - Some occurrences of modeled stratospheric ozone intrusion when none observed (and vice versa)
- Underestimation of JPAD winter high ozone and highest ozone in California
  - Model not configured for simulating cold pooling
  - Coarse (12 km) grid limits urban ozone simulation, especially in marine environment

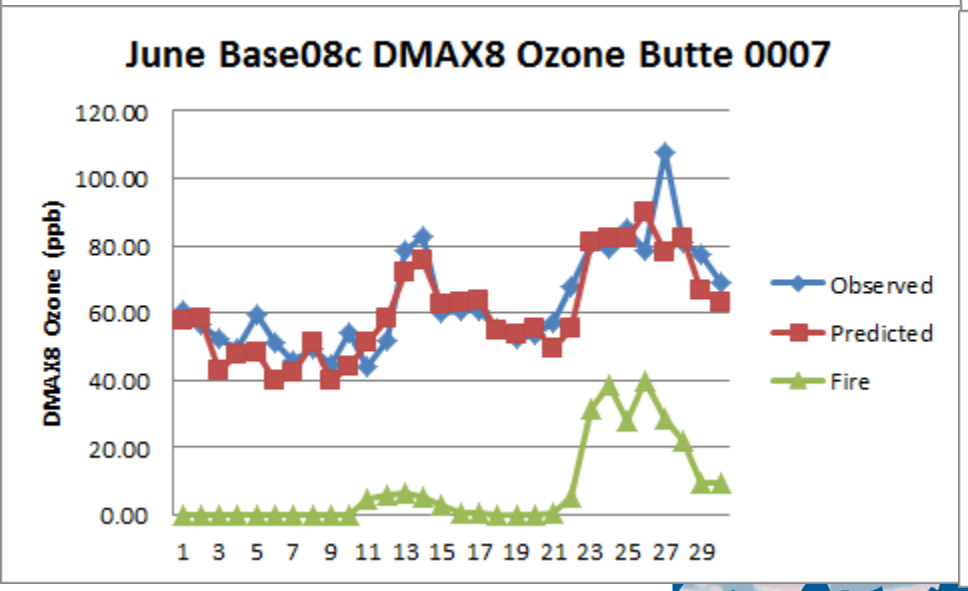
Example Daily Max 8-Hr Ozone Time Series

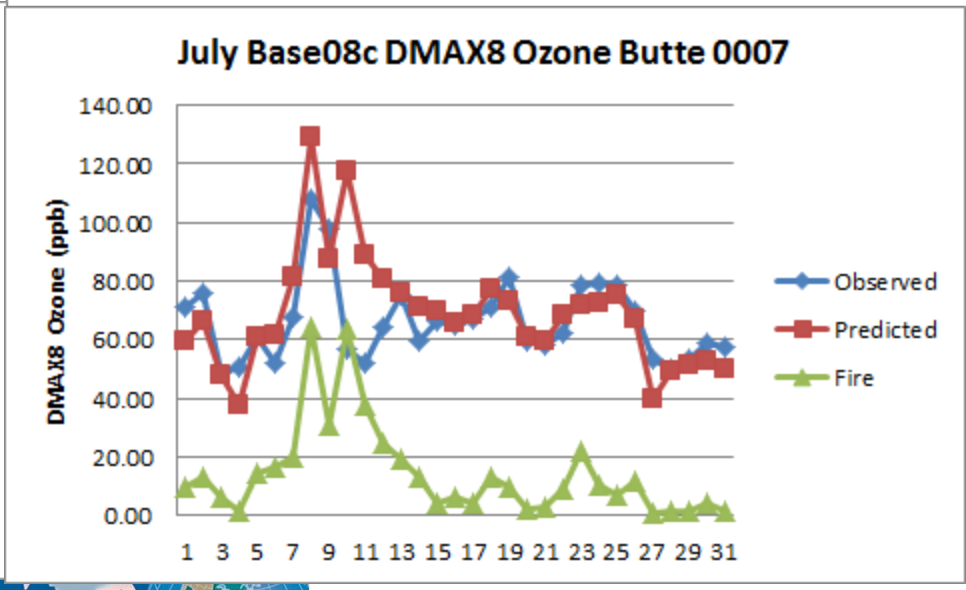
- Northern California June and July 2008
  - Dry lightning on June 21 ignited multiple wildfires
- Gothic, CO CASTNet Apr, May, Jul & Aug
  - High terrain monitor susceptible to stratospheric ozone intrusion
- Glacier, MT CASTNet Jun-Aug
  - Why do we have MT ozone overestimation bias?
- Denver Ozone Monitors July 2008
  - Several high ozone episodes

Northern California Wildfires Jun-Jul 2008

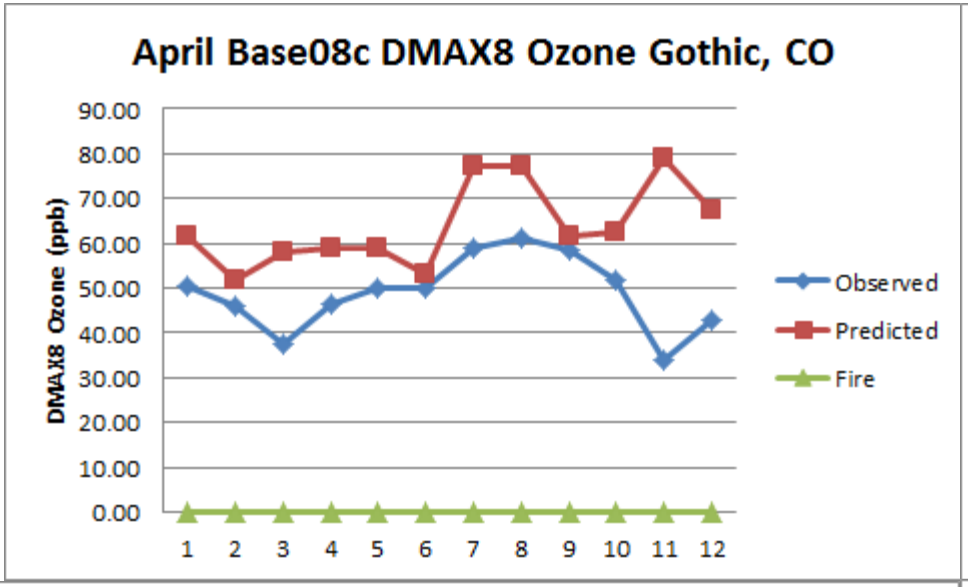


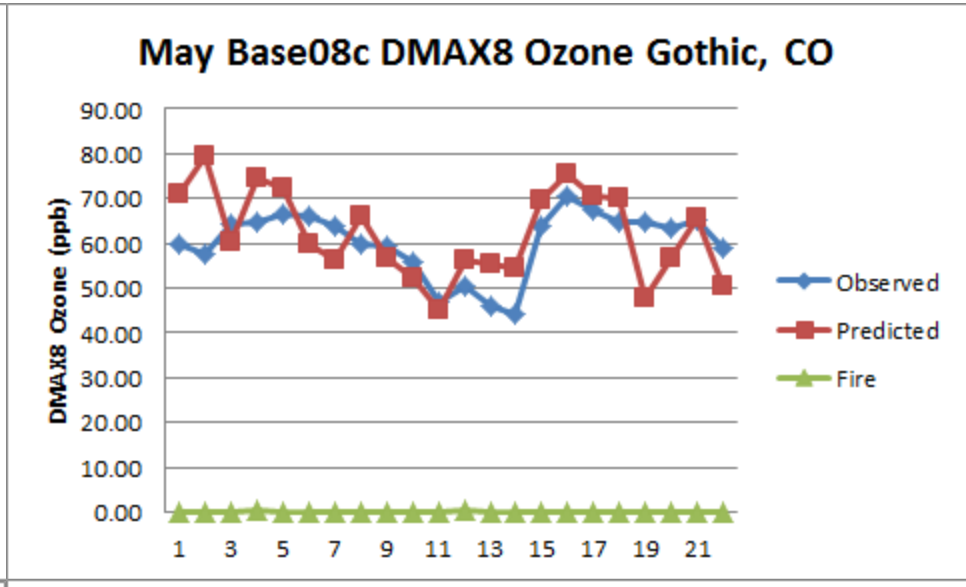


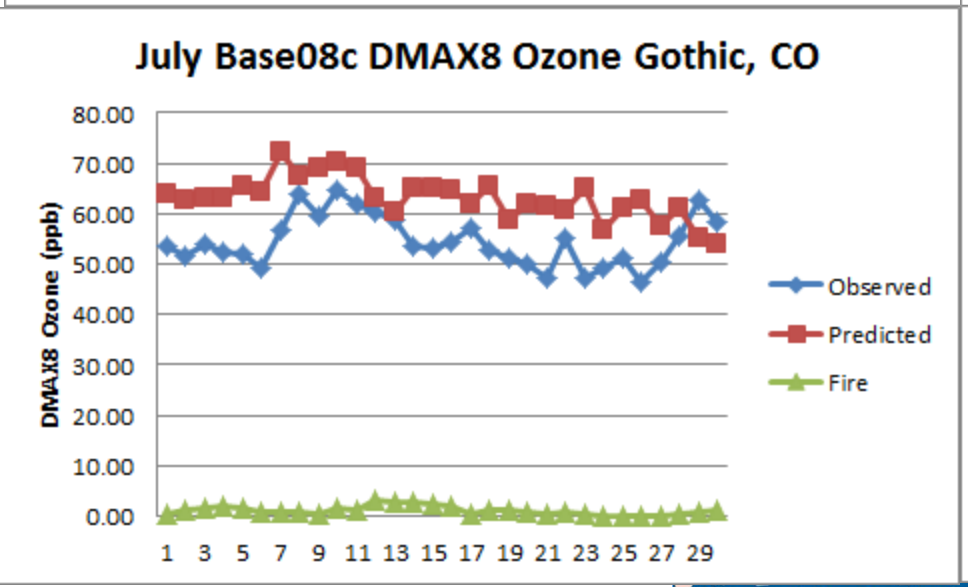


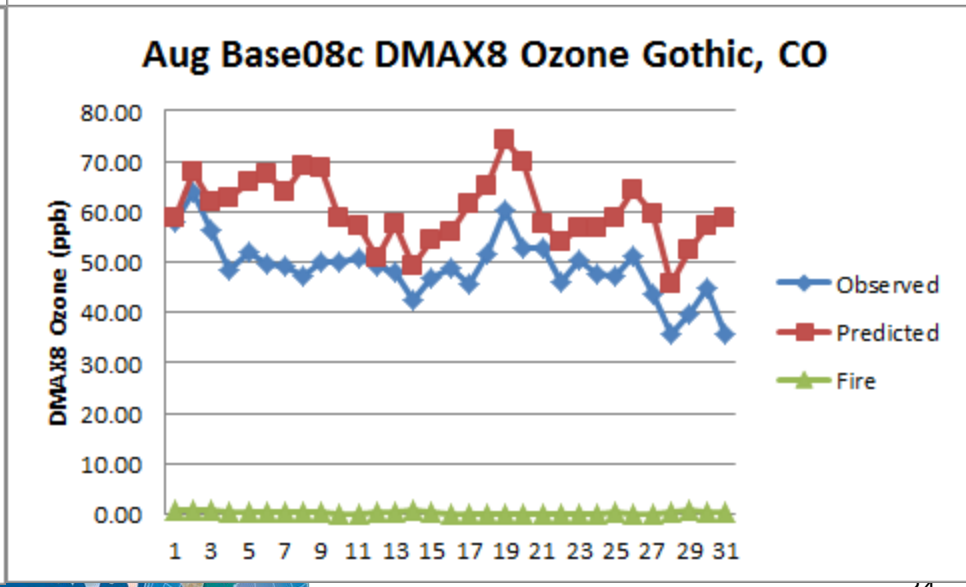


Gothic, CO CASTNet Site

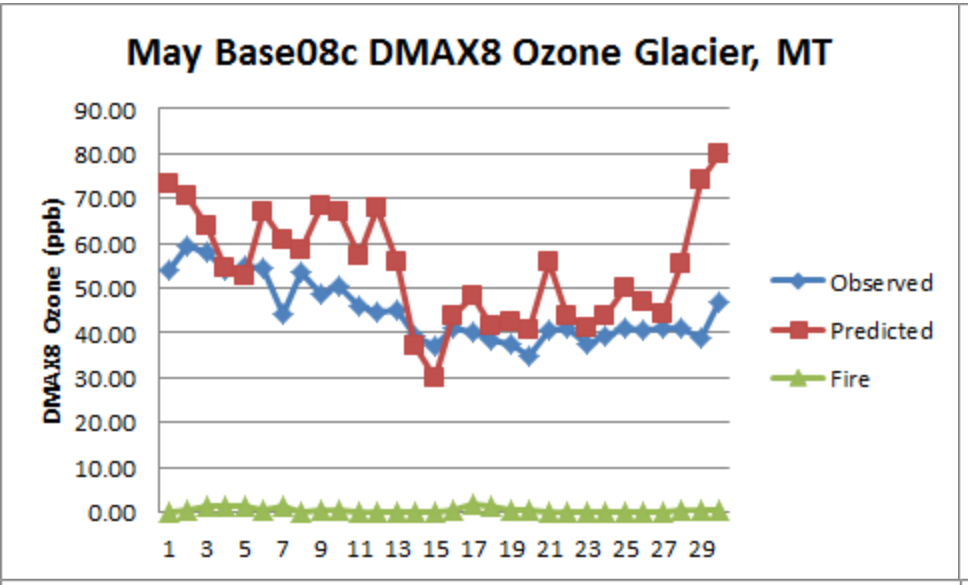


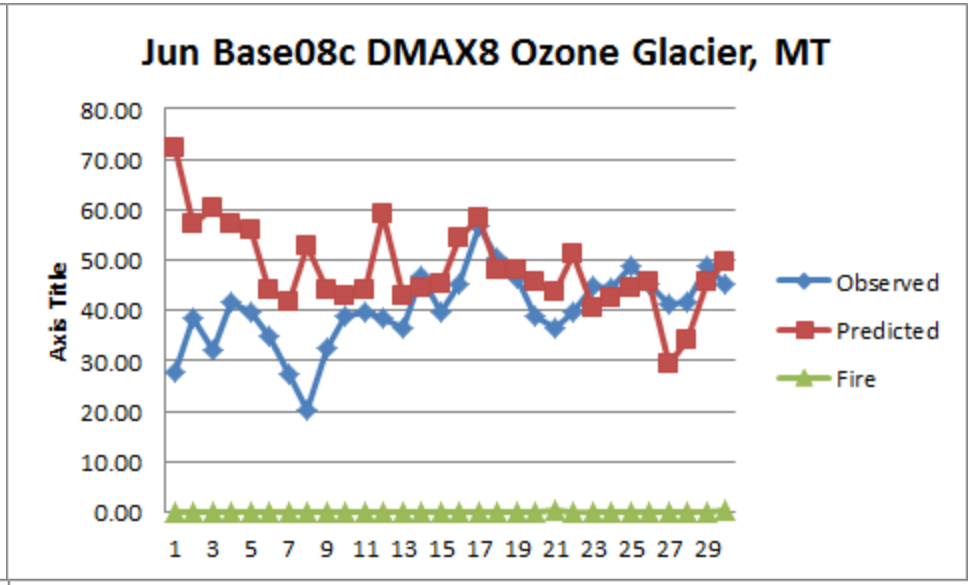


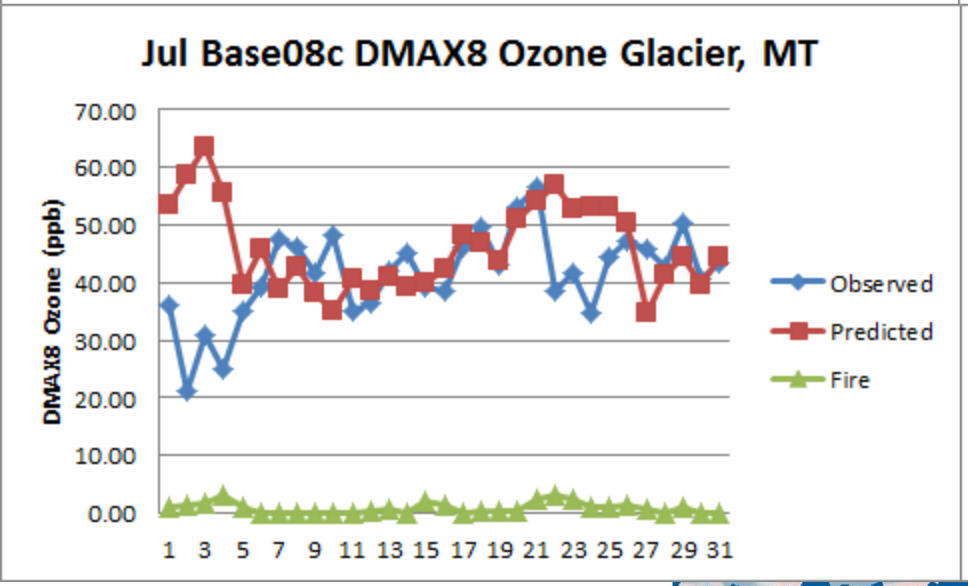


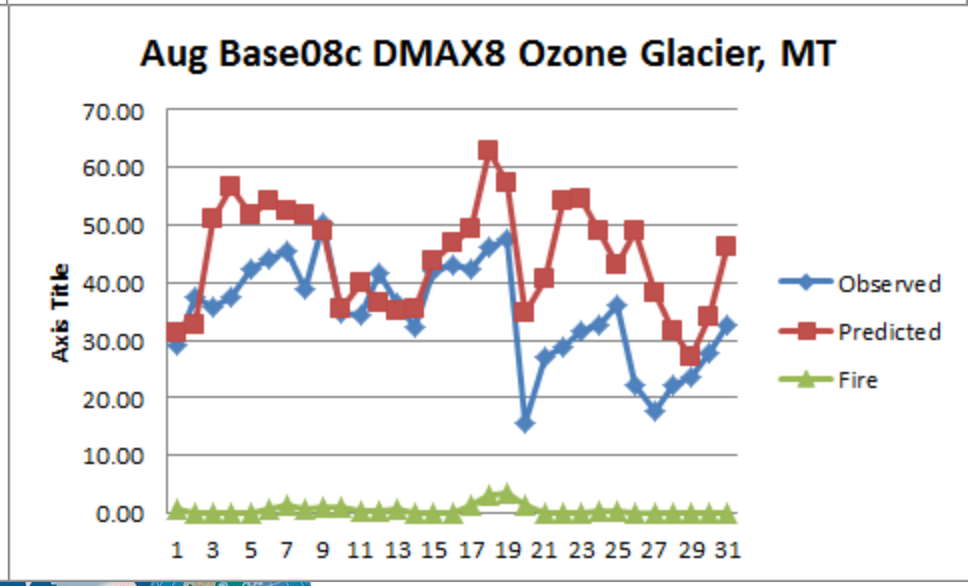


Glacier, MT CASTNet Site

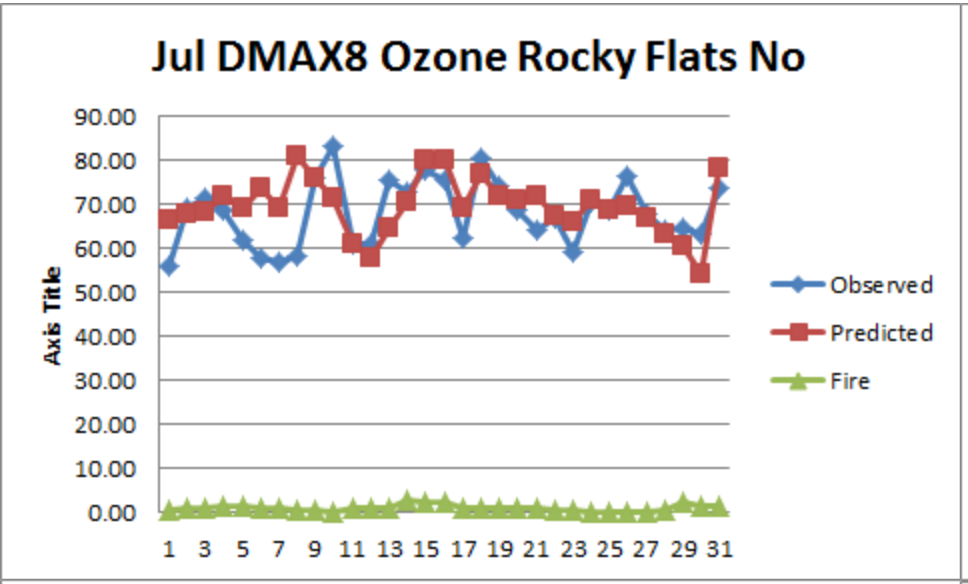


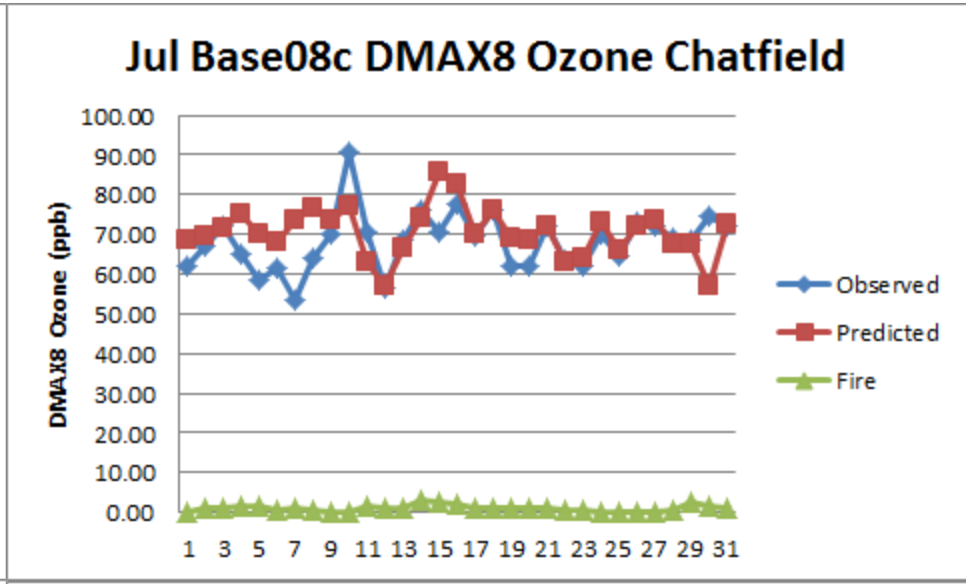


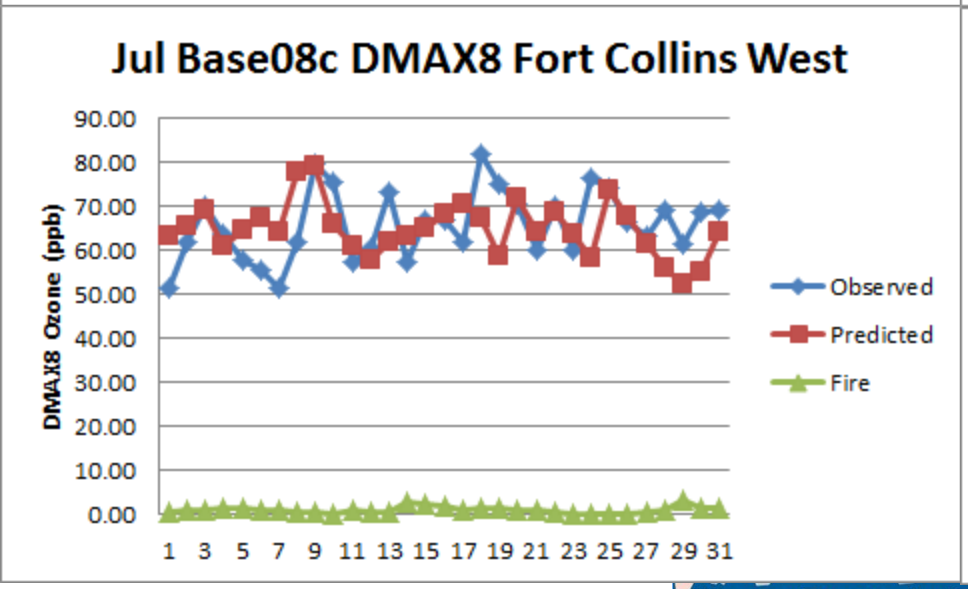


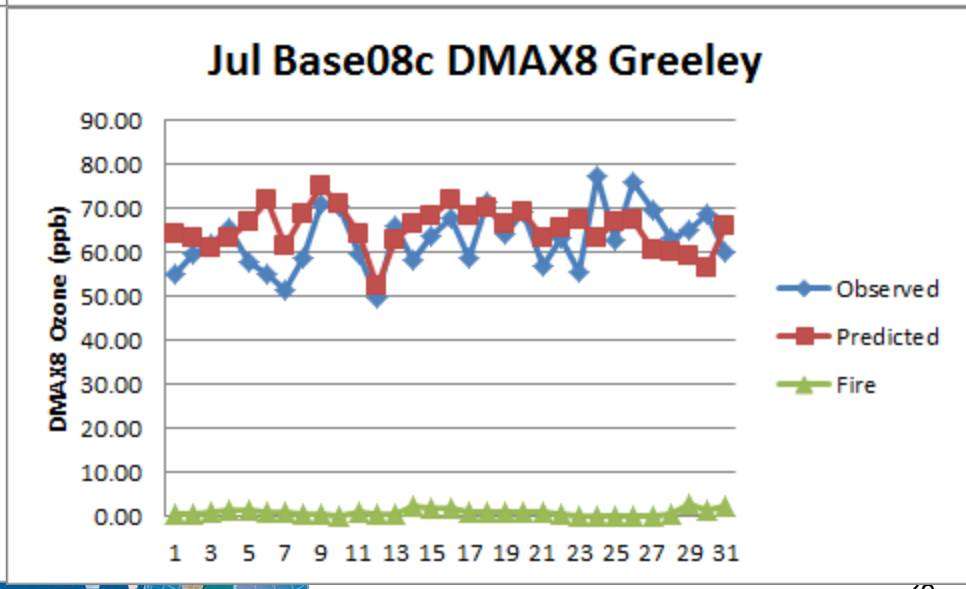


Denver Ozone Monitors July 2008









Next Steps Ozone Model Performance

- Continue analyzing ozone model performance results
- Performing MOZART vs. GEOS-Chem 36 km CONUS Boundary Condition (BC) sensitivity test
  - Tracking ozone from BCs at three vertical levels:
    - Clearly stratospheric ozone (upper levels)
    - Clearly tropospheric ozone (lower levels)
    - In between (middle levels)
  - Determine whether GEOS-Chem does better job in estimating stratospheric ozone intrusion and reduces ozone positive bias
- After performing simulation for 4 km Detailed Source Apportionment Domain (DSAD) analyze 4 km ozone performance and compare with 12 km results

Base08c Particulate Matter Model Performance

- Total $PM_{2.5}$ Mass
  - FRM, CSN and IMPROVE monitoring networks
- Speciated: SO4, NO3, NH4, EC, OA, Soil, OPM2.5, PMC
  - CSN, IMPROVE, CASTNet and NADP
  - Soil & OPM25 two measures of other PM2.5
- PM Model Performance Goals and Criteria from RPOs

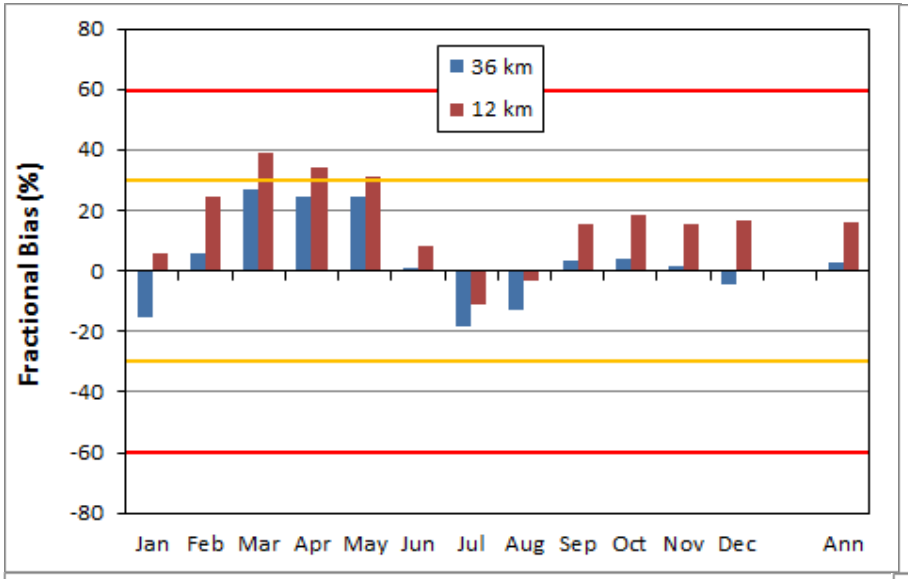
	Fractional Bias (FB)	Fractional Error (FE)
Ozone Performance Goal	≤±15%	≤35%
PM Performance Goal	≤±30%	≤50%
PM Performance Criteria	≤±60%	≤75%

Base08c PM Model Performance

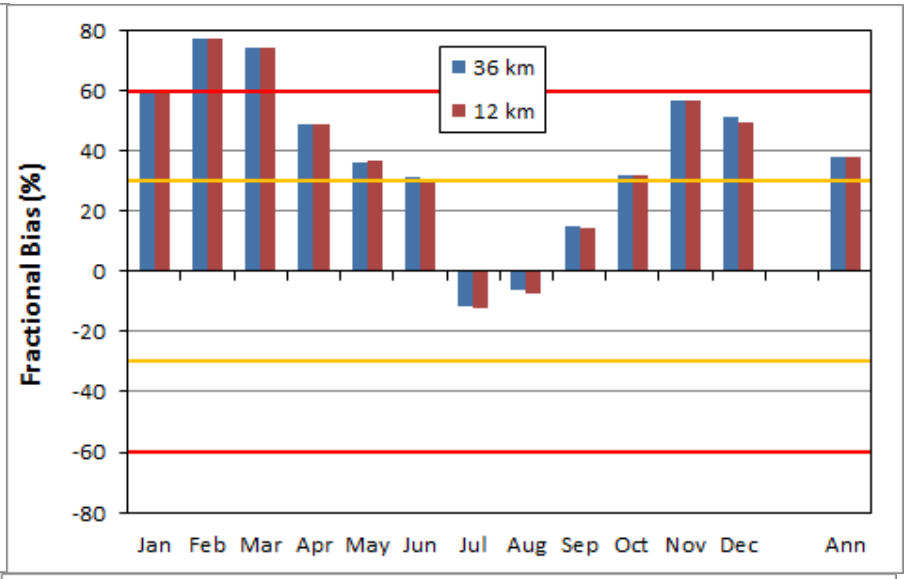
- CAMx 2008 36 and 12 km Base08c PM model performance across 12 km WESTUS domain and comparison with PM performance goals and criteria
- Bar Charts of monthly and annual Fractional Bias (FB) and Fractional Error (FE) across CSN (urban) and IMPROVE (rural) monitoring sites in the 12 km WESTUS domain for total $PM_{2.5}$ mass and speciated $PM_{2.5}$

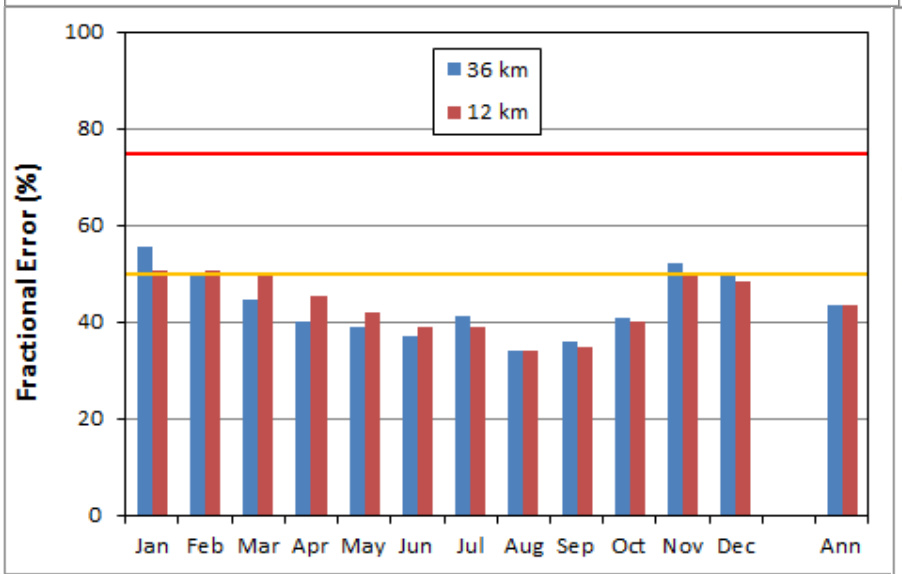
Total $PM_{2.5}$ Mass 12 km WESTUS

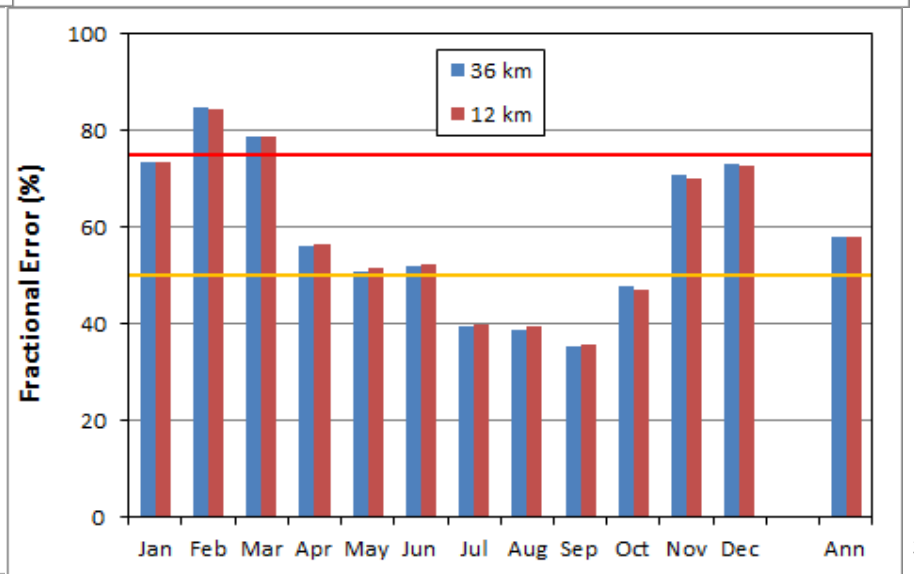
CSN



IMPROVE



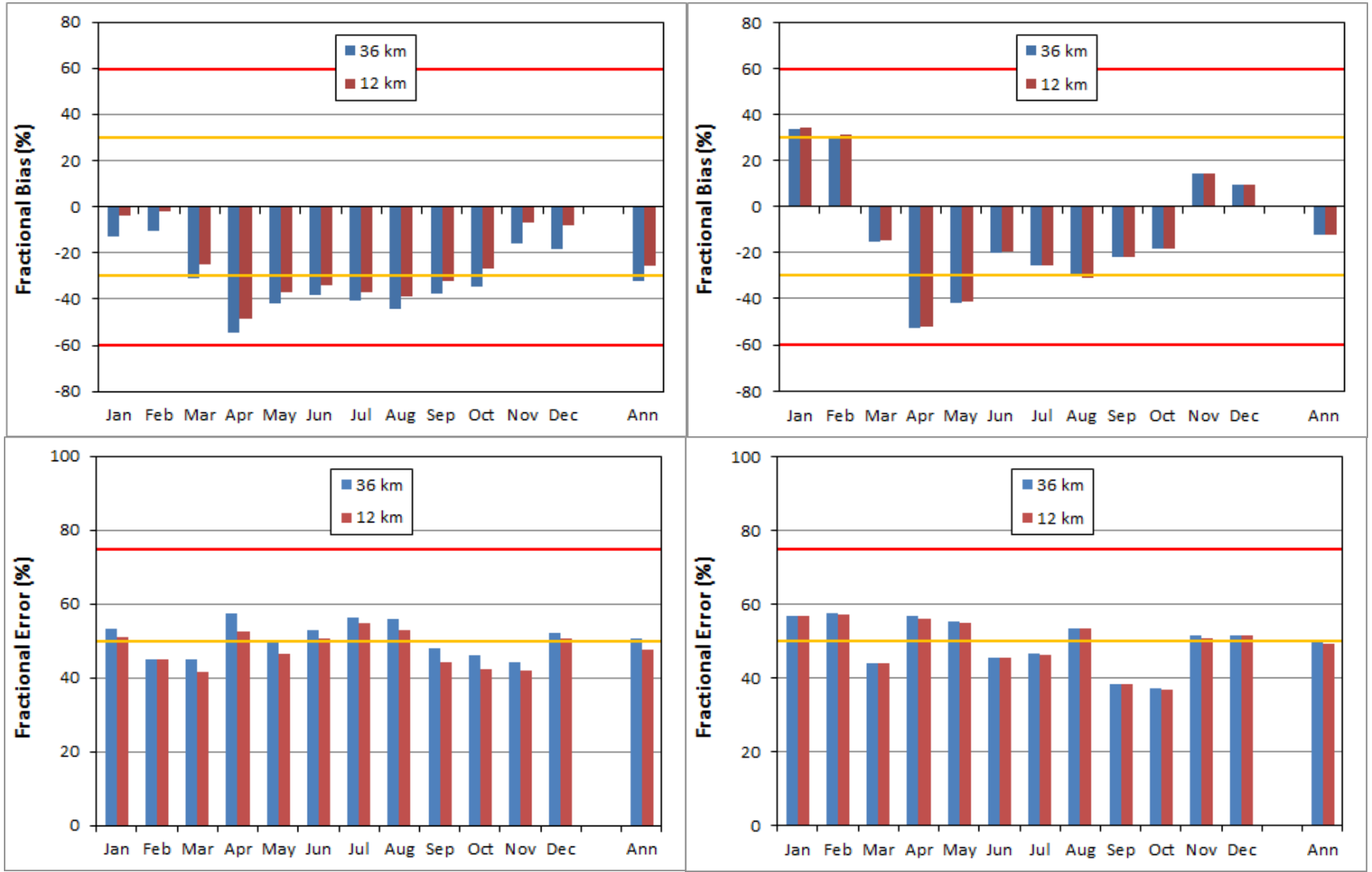




Sulfate (SO4) 12 km WESTUS

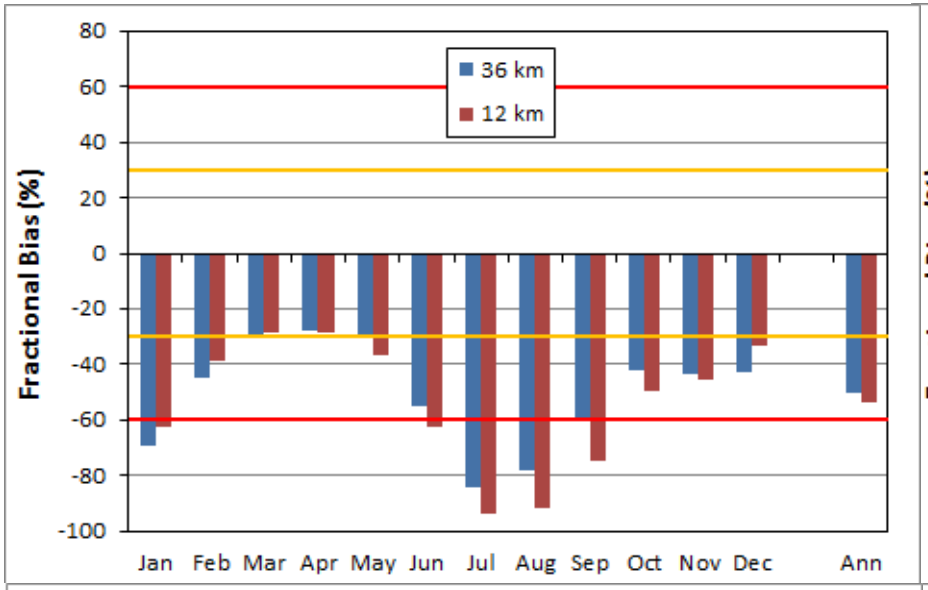
CSN

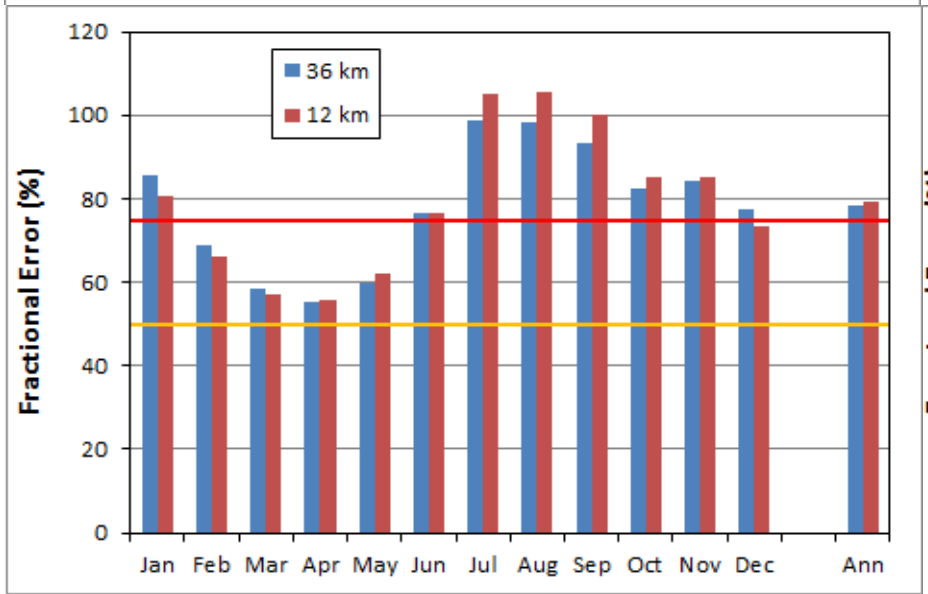
IMPROVE



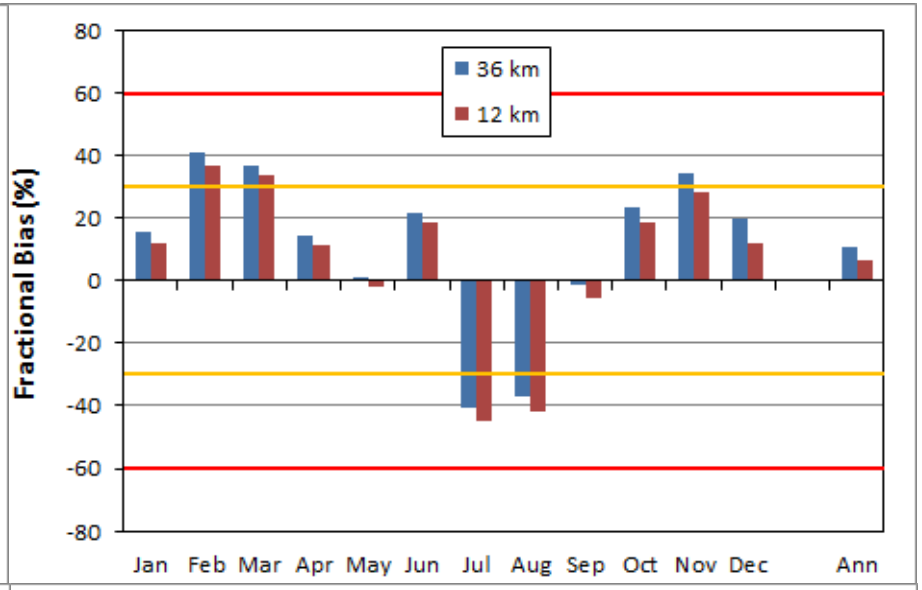
Nitrate (NO3) 12 km WESTUS

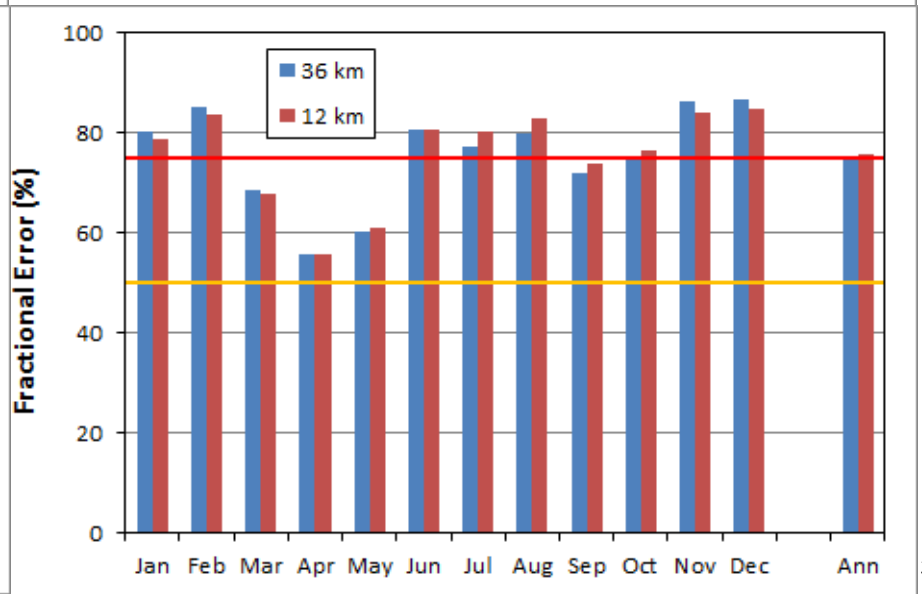
CSN





IMPROVE

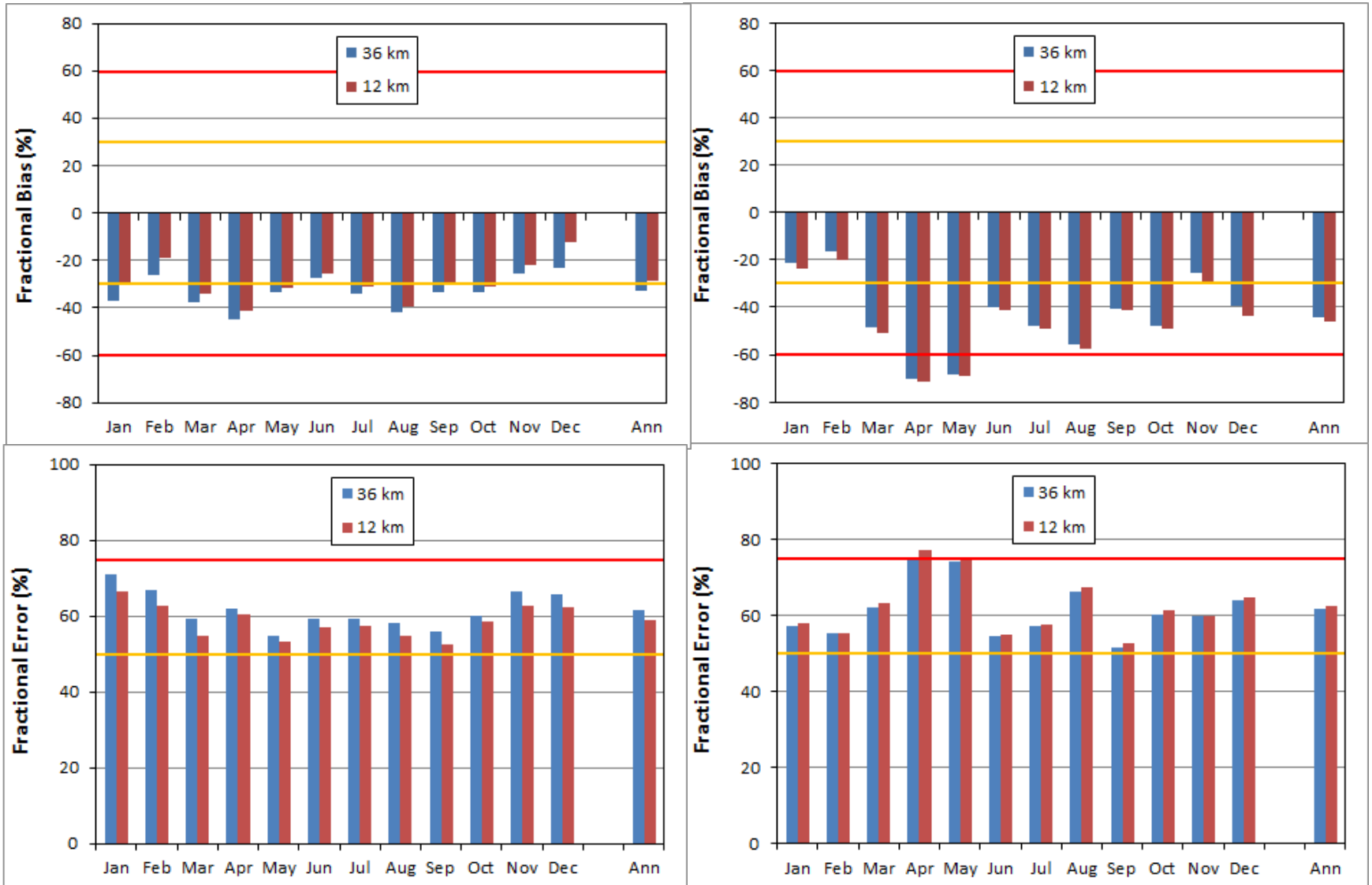




Ammonium (NH4) 12 km WESTUS

CSN

IMPROVE (NH4d)

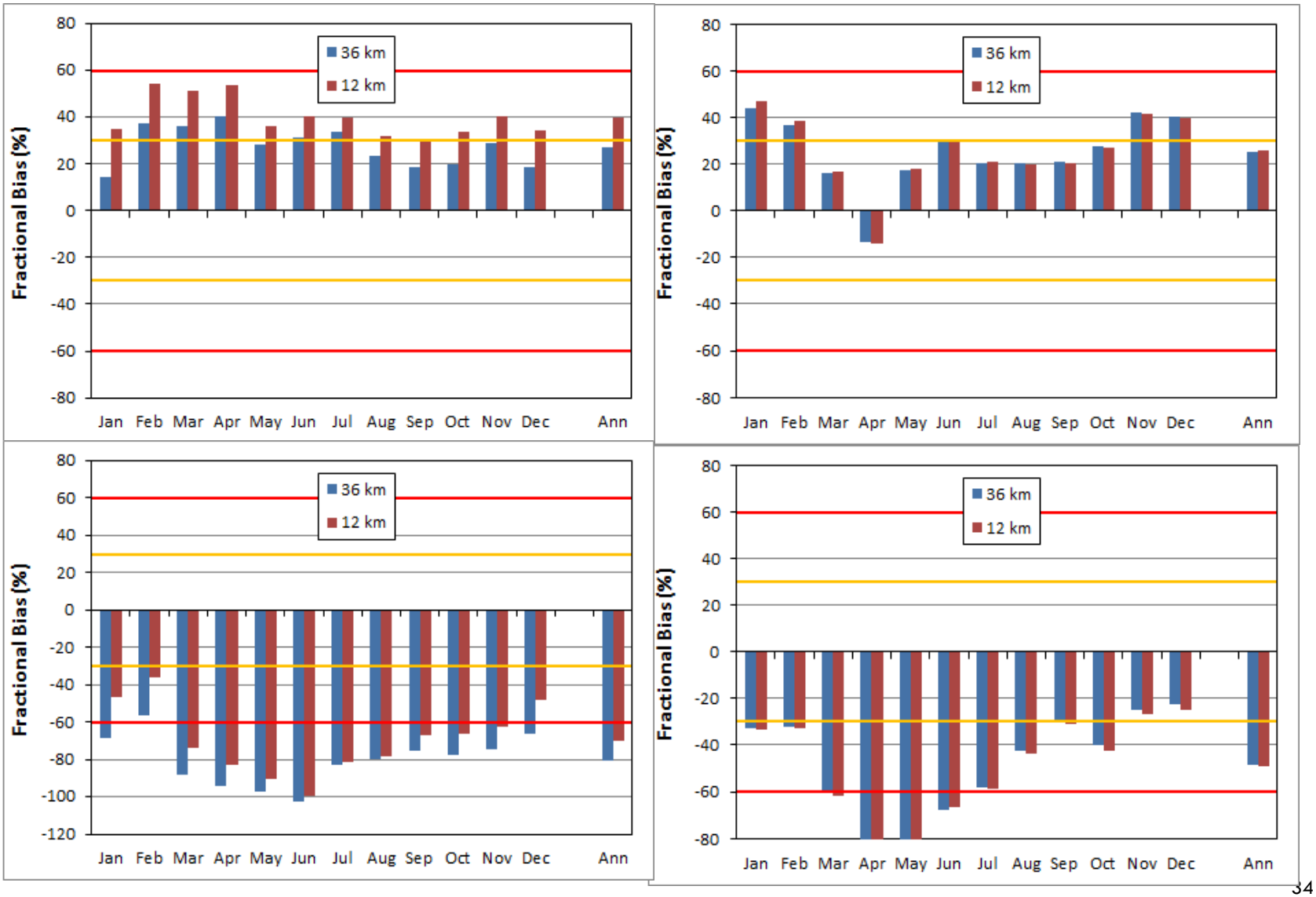


Elemental Carbon (EC) and Organic Aerosol (OA)

CSN | IMPROVE

EC

OA



Two different ways of looking at Other PM2.5

- Observed
  - Soil = 3.73*Si + 1.63*Ca + 2.42*Fe + 1.94*Ti
  - OPM2.5 = PM2.5 – (SO4+NO3+NH4+EC+OA)
    - If OPM2.5 is negative it is set to zero, which happens fairly frequently
- Modeled
  - PMFINE = all PM2.5 not explicitly speciated into SO4, NO3, NH4, EC or OA in the emissions modeling
- Different PM measurement techniques have different measurement artifacts

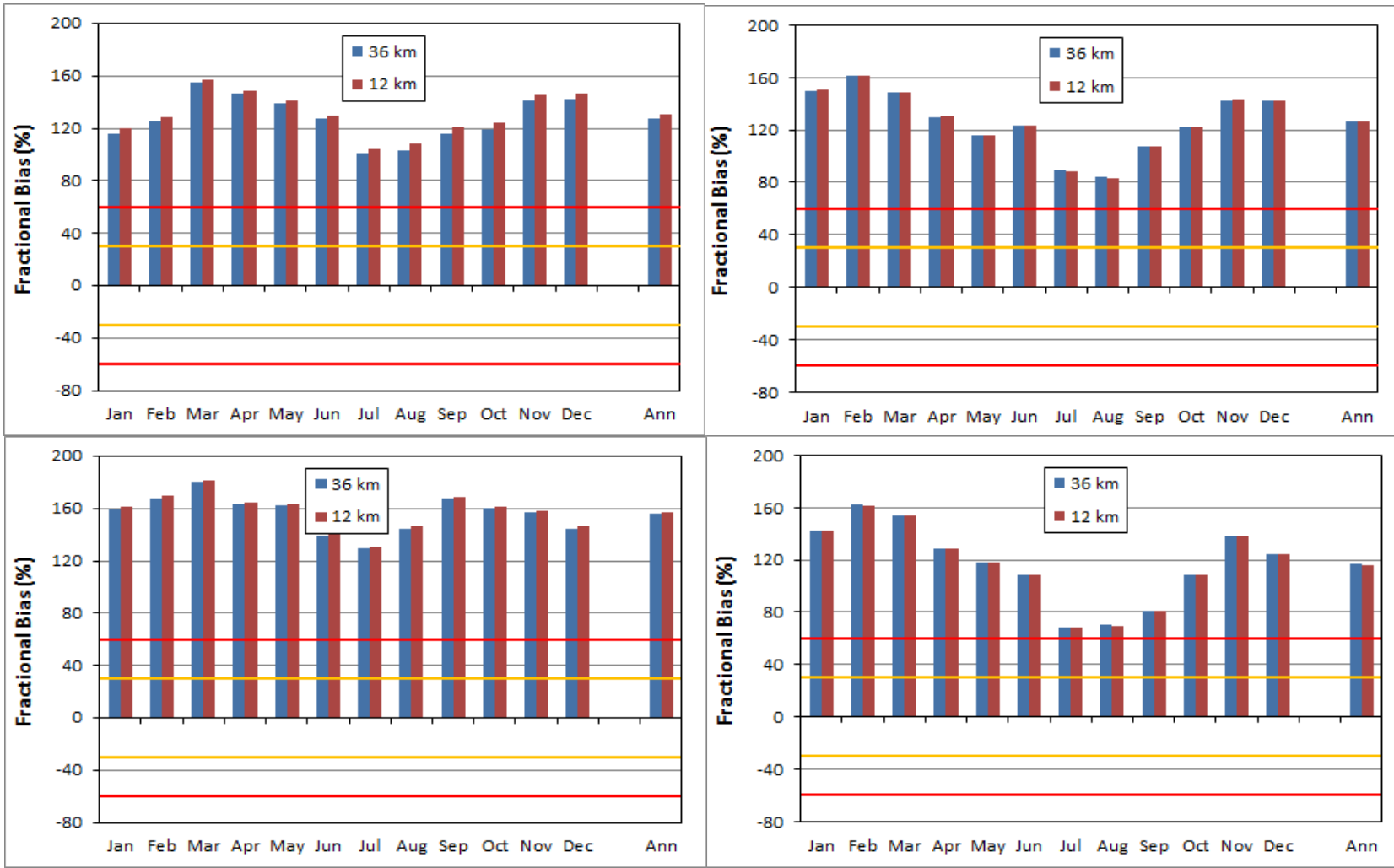
Other PM2.5 WESTUS 12 km Domain

CSN

IMPROVE

Soil

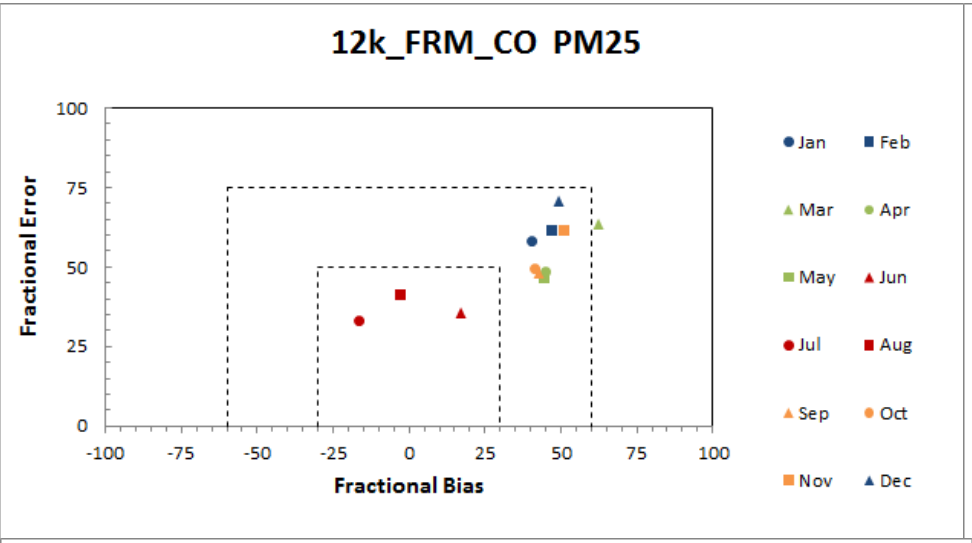
OPM2.5

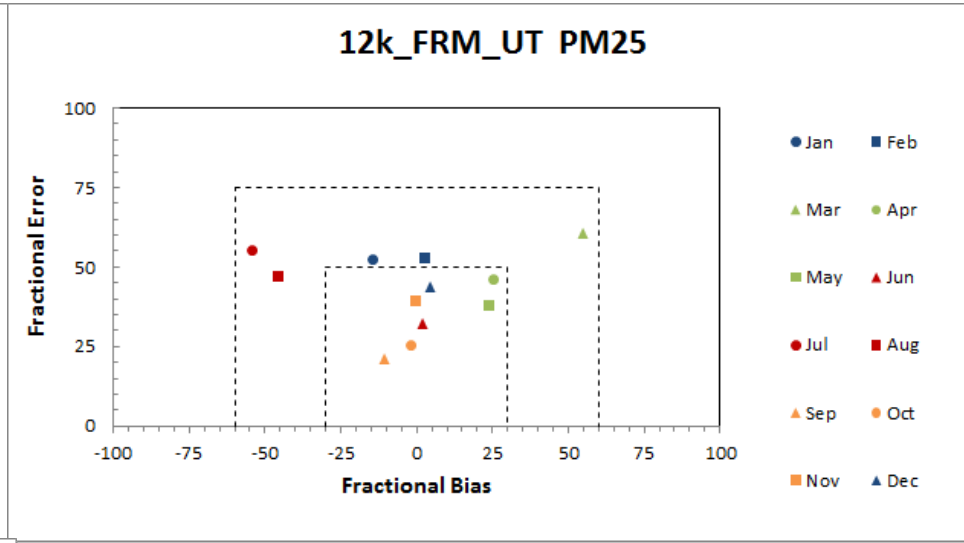


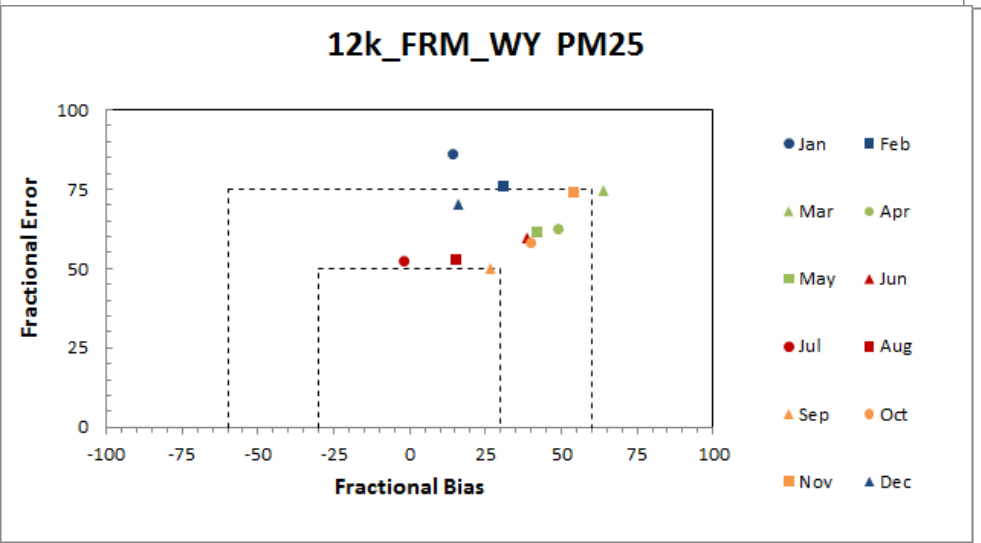
PM Model Performance using Soccer Plots

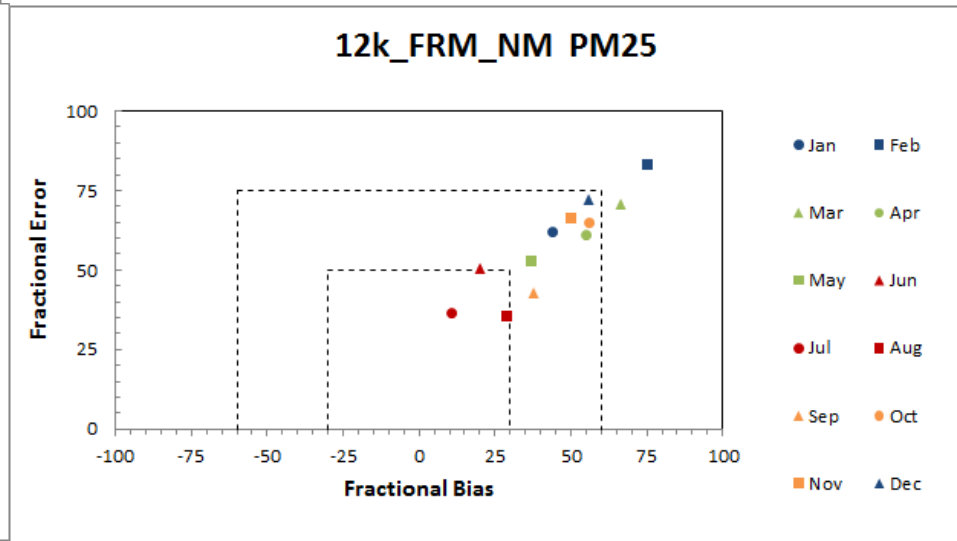
- Soccer Plots are scatter plots that plot monthly Fractional Bias (FB: x-axis) versus Fractional Error (FE: y-axis) with the PM Model Performance Goals and Criteria represented as boxes
- If the FB/FE monthly point falls within the Performance Goal and/or Criteria box that that benchmark is achieved
- Separate Soccer Plot for each western State and PM species
- Examples focus on Colorado
- Note that x/y axis scale in Soccer Plots can vary but Goals/Criteria boxes represent same values

CAMx Base08c FRM $PM_{2.5}$ MPE: CO, UT, WY & NM

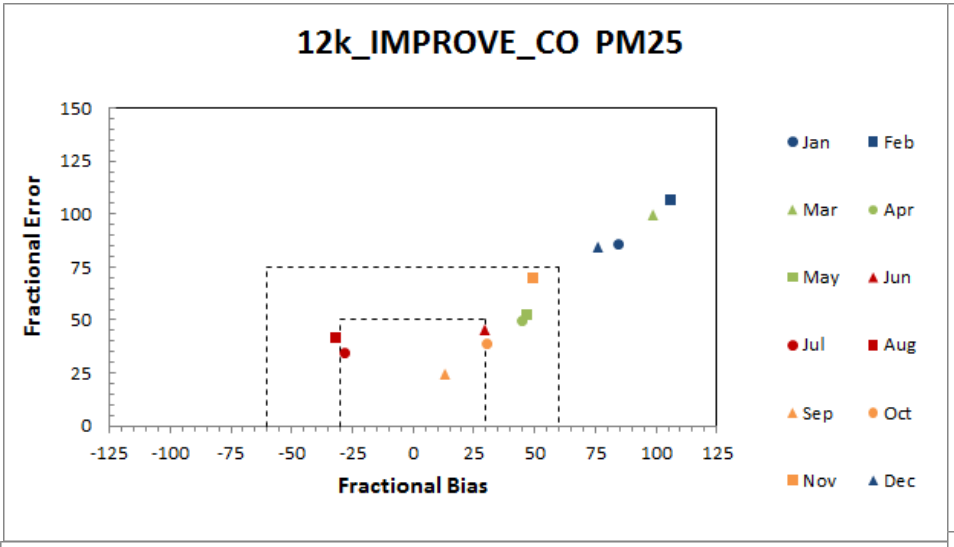


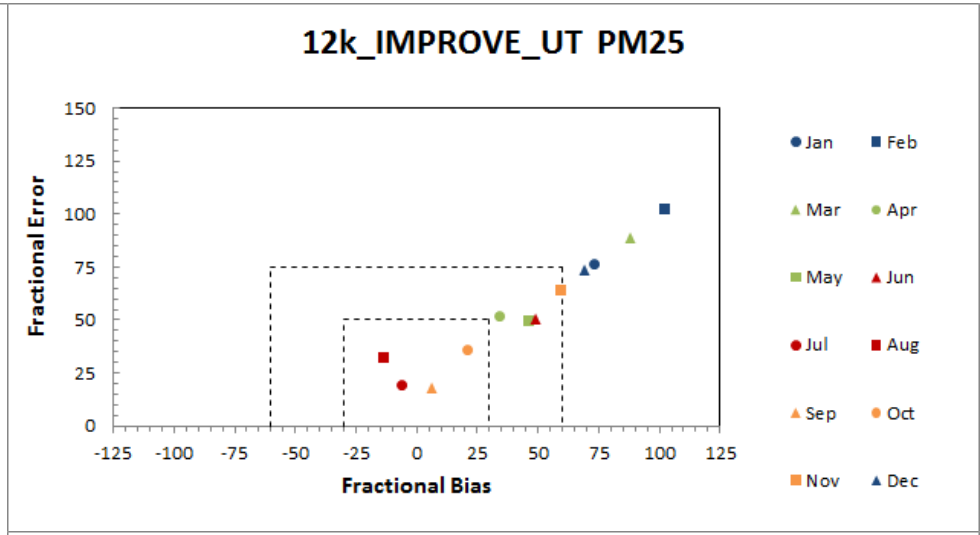


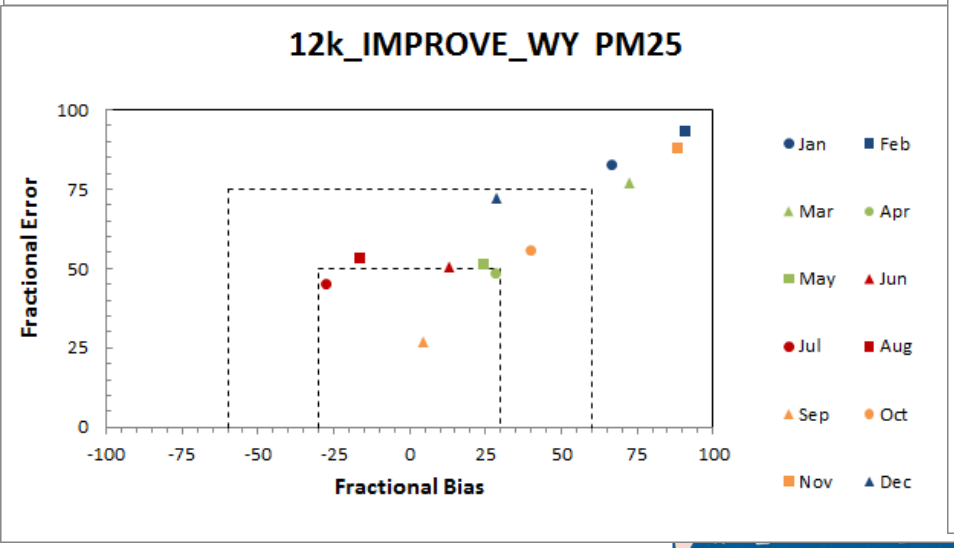


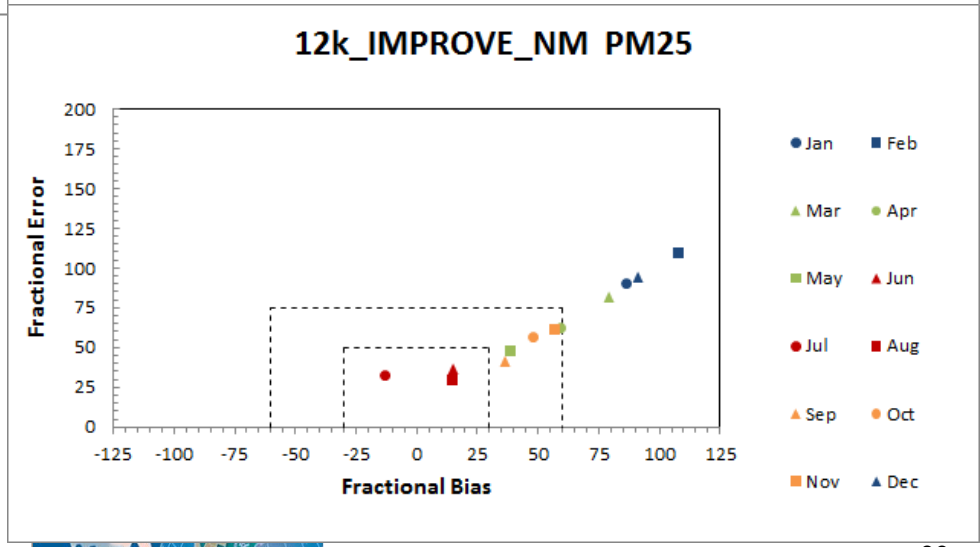


CAMx Base08c IMPROVE $PM_{2.5}$ MPE: CO, UT, WY & NM

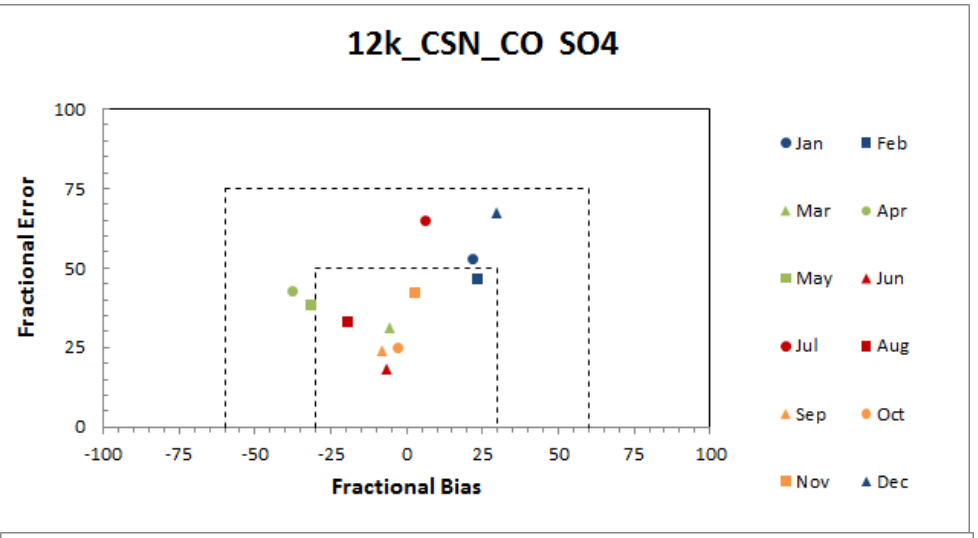




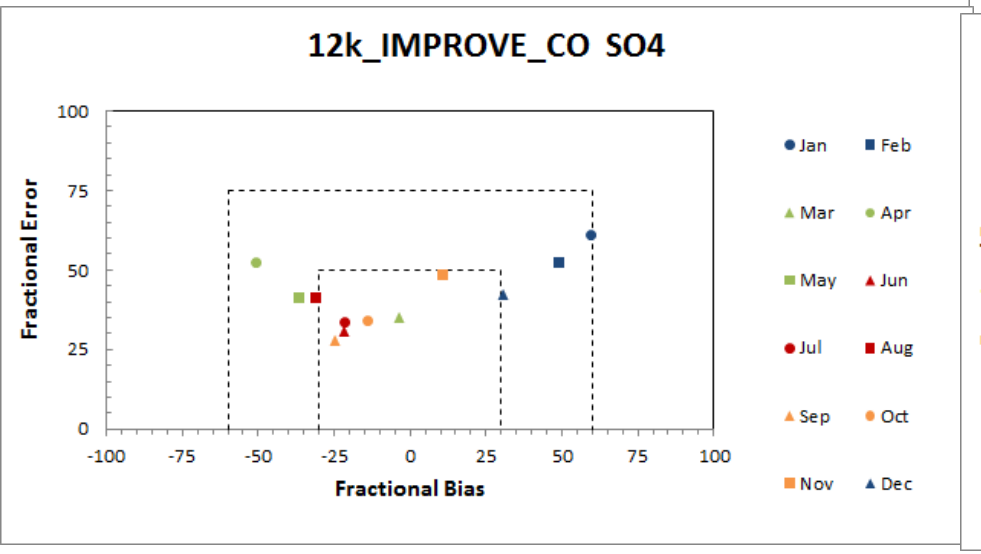


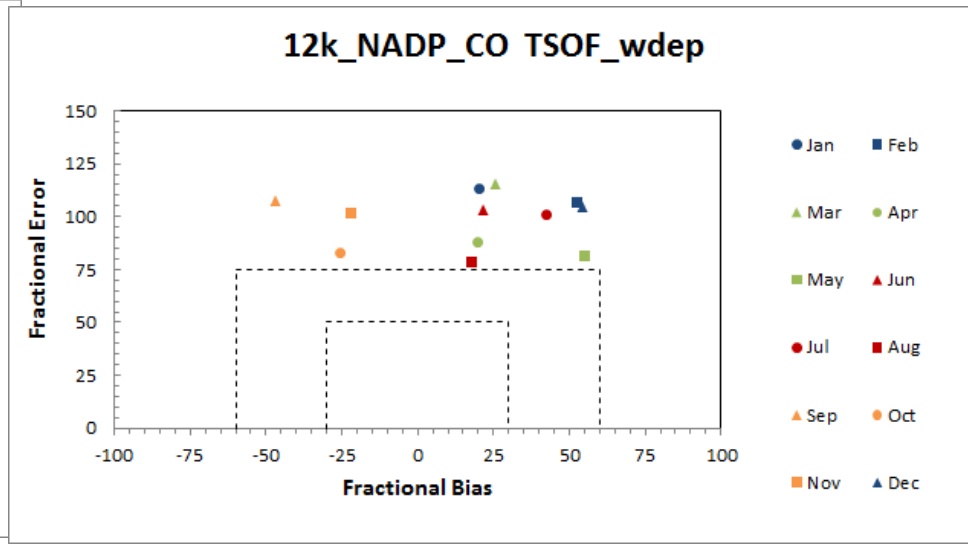


Colorado Sulfate (SO4) Performance

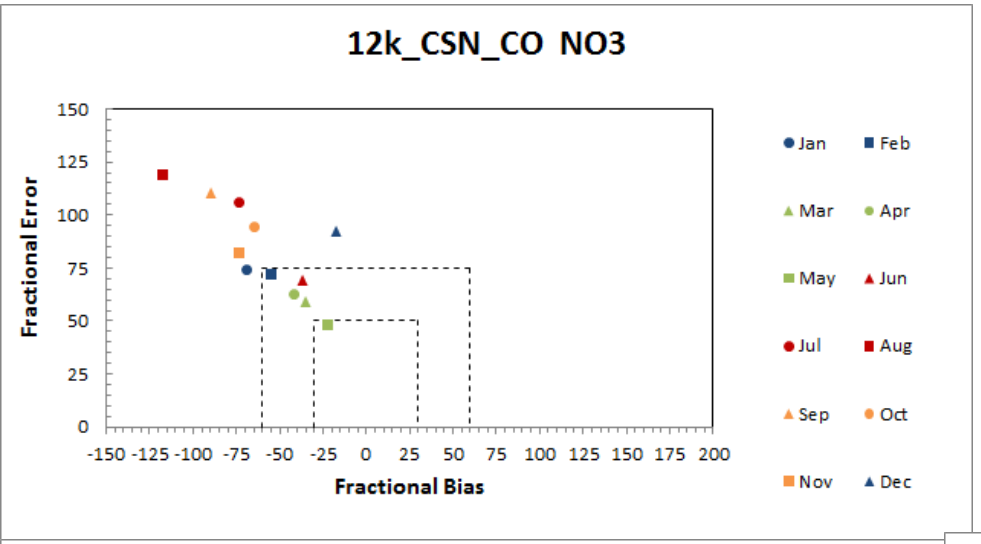


- Generally good SO4 performance slight overestimation in cold months
- Wet SO4 deposition bias reasonable with slight overestimation and error in 75-125% range

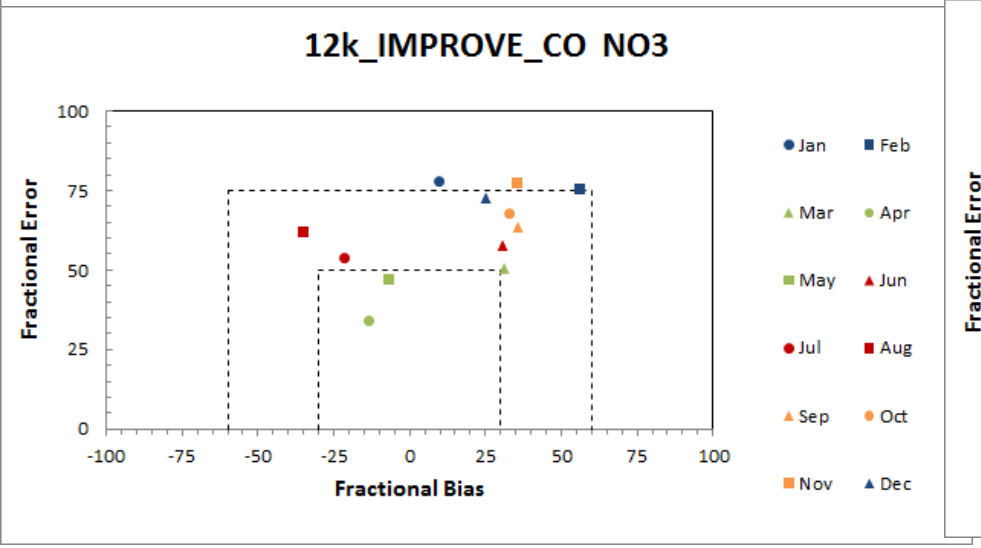


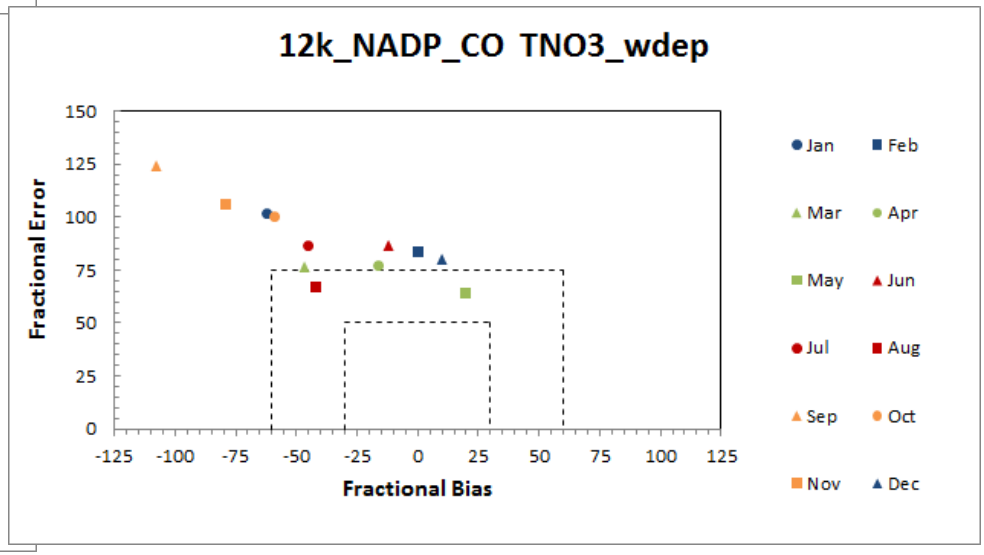


Colorado Nitrate (NO3) Performance

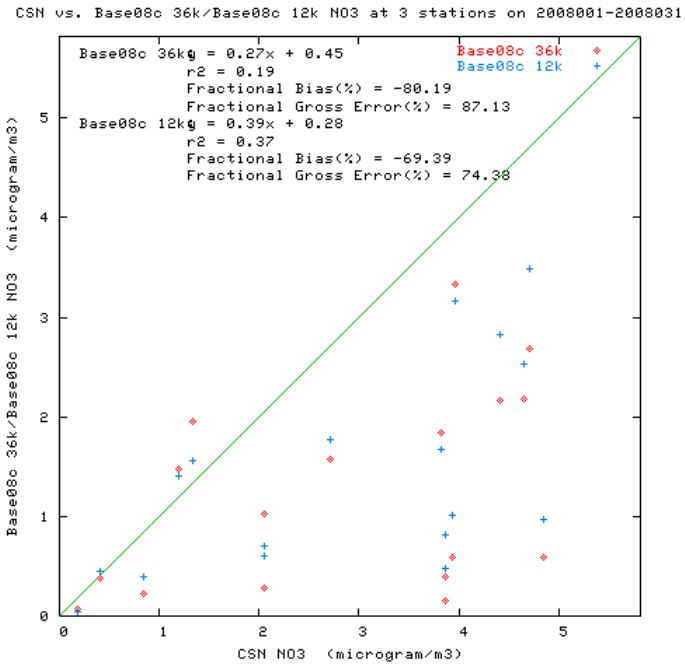


- Summer NO3 underestimation bias at CSN & NADP



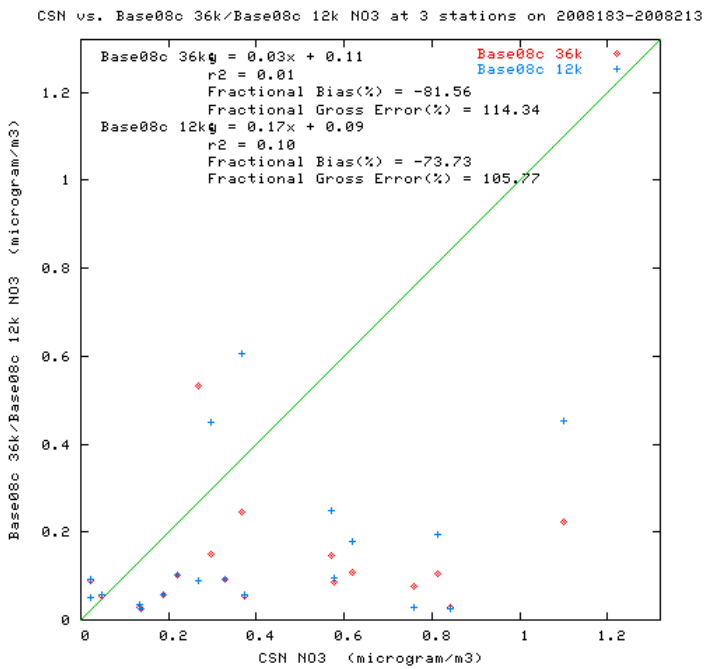


CO NO3 Performance



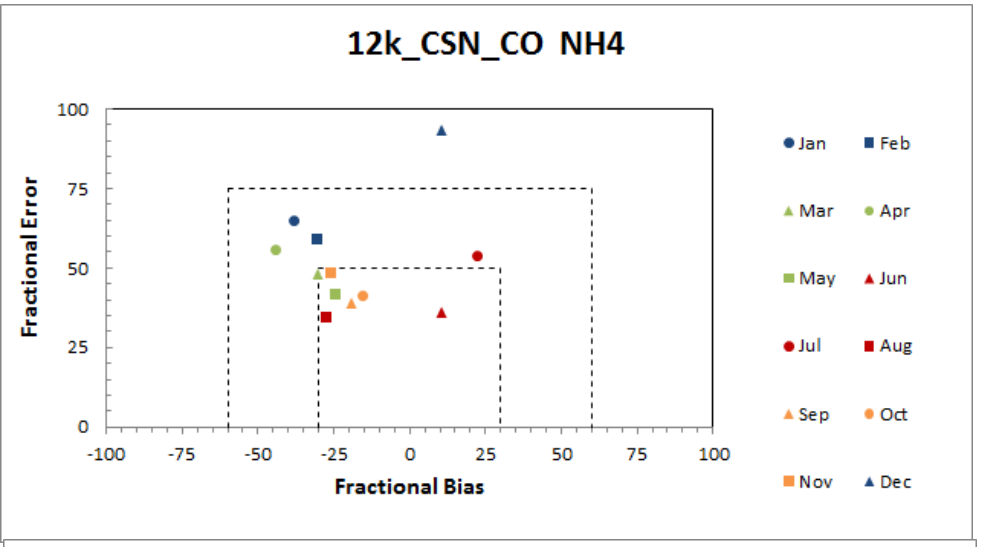
← January CSN

- Summer NO3 underestimation occurs when observed NO3 very low and not important component of $PM_{2.5}$ or visibility
- In past some improvements seen by including mineral nitrate to lift modeled NO3 away from zero

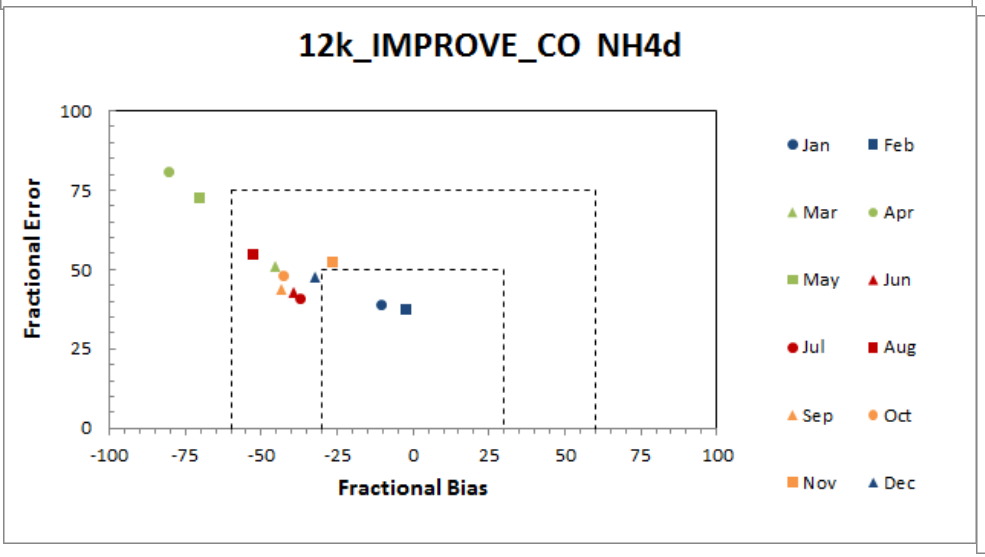


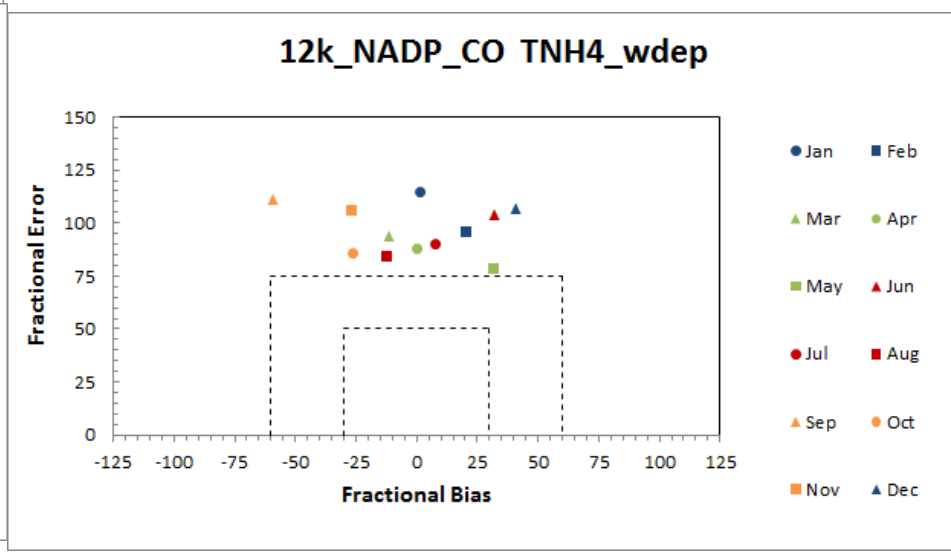
← July CSN

Colorado Ammonium (NH4) Performance

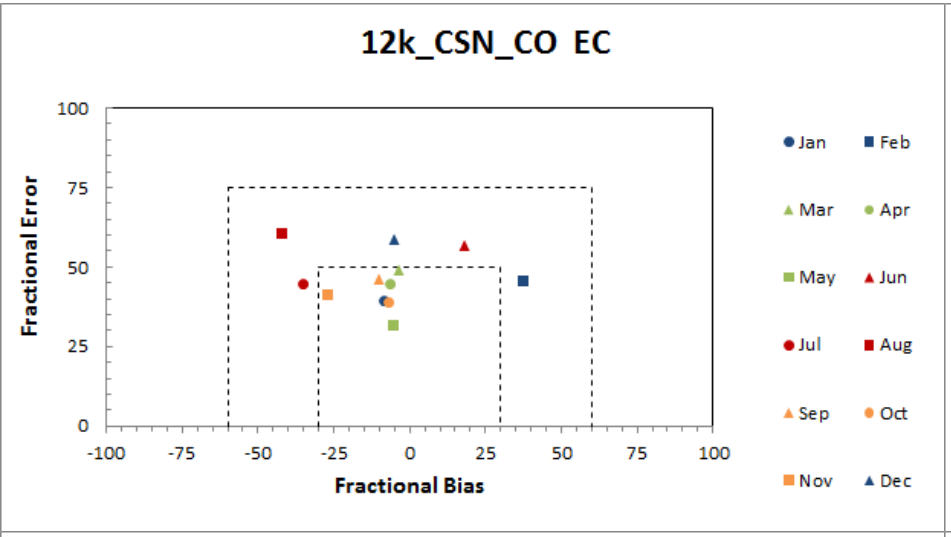


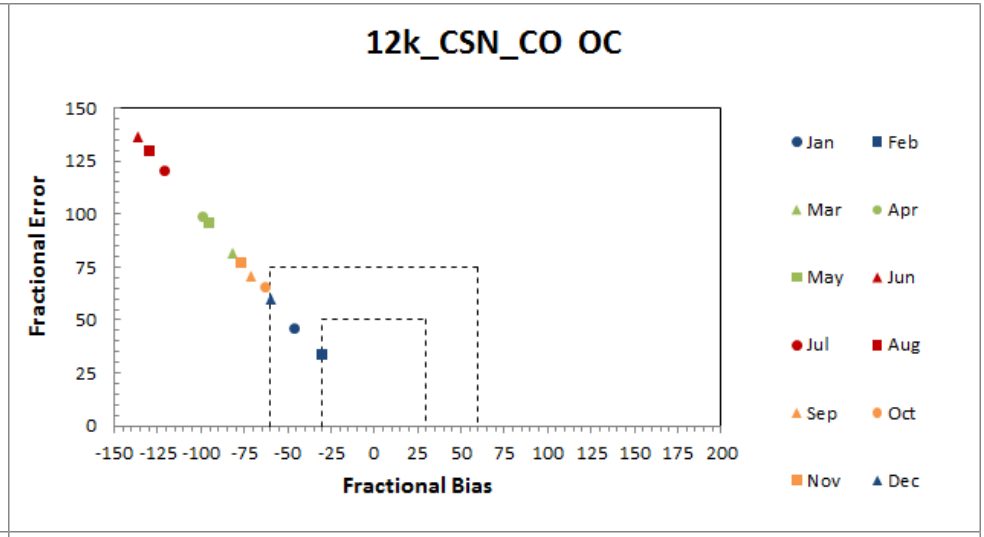
- NH4 performance tied to SO4 and NO3
- IMPROVE uses derived NH4 (NH4d) assuming SO4 & NO3 are completely neutralized so underestimation expected

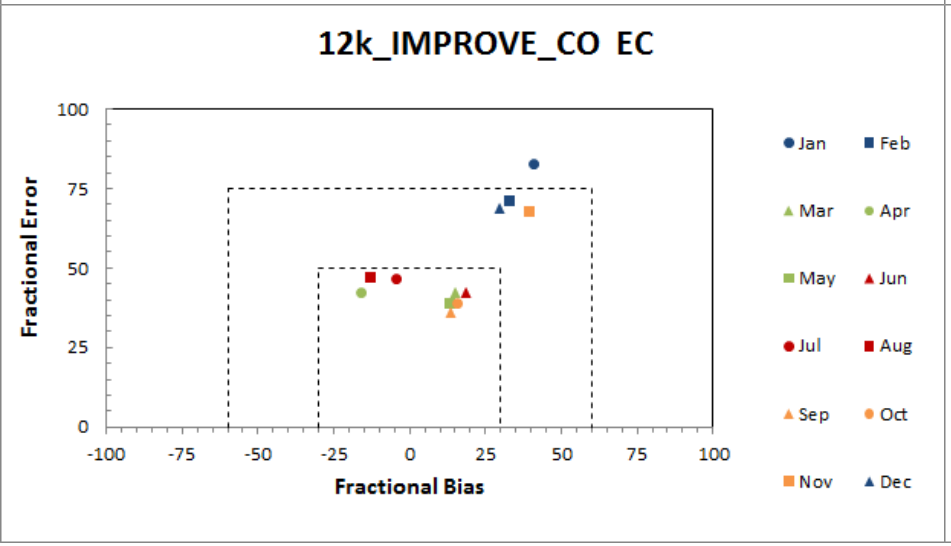


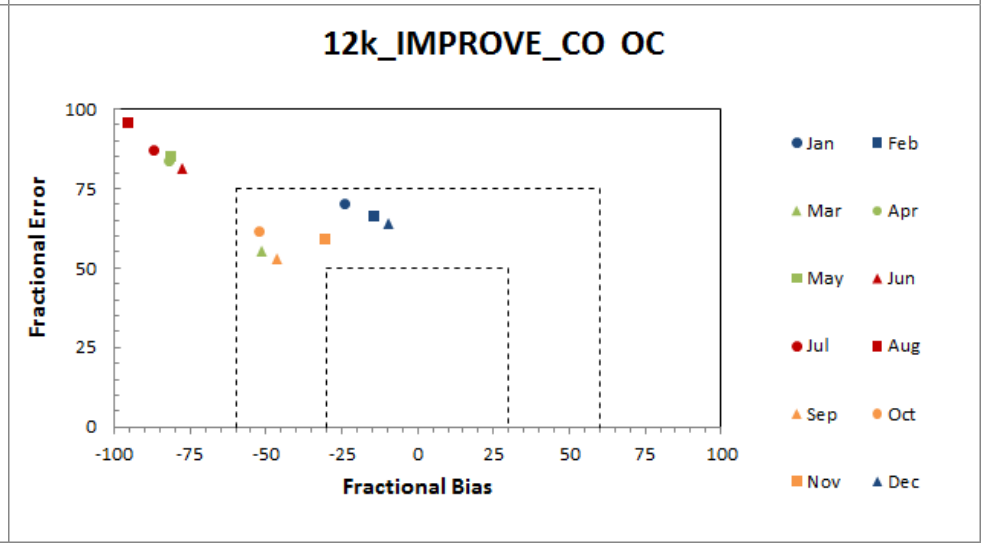


Colorado EC and OA (=1.4xOC) Performance









Summary Base08c CAMx PM Performance

- There appear to be operational difference on how the speciated PM species are defined in the networks and modeled vs. monitoring
- In general PM2.5, SO4, NH4 and EC performance is reasonably good
- NO3 underestimation in summer when concentrations are very low
- OA is underestimated especially in summer and OPM2.5 is overestimated year-round

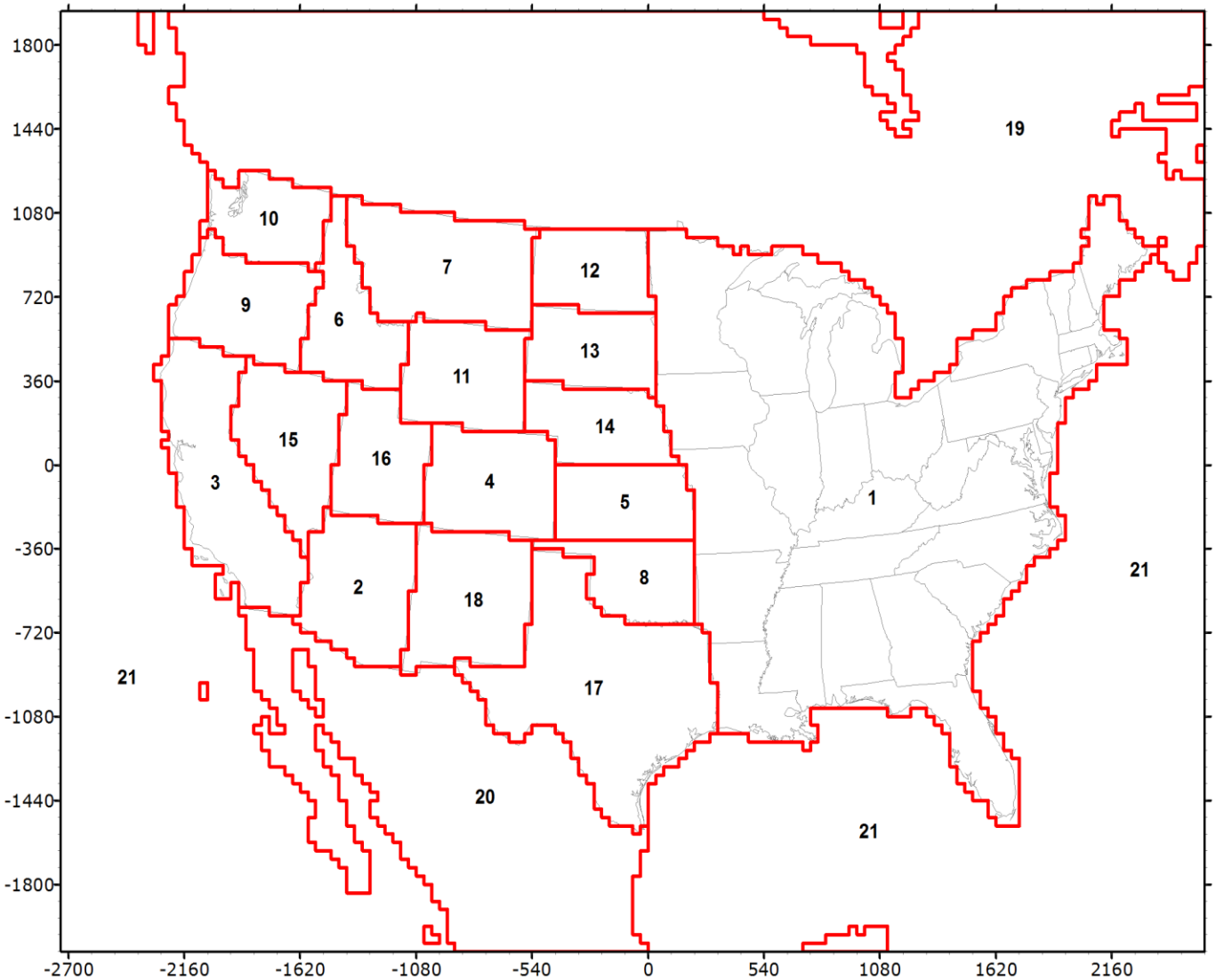
Summary Base08c CAMx PM Performance

- Potential OA underestimation causes:
  - Monitoring artifacts and model/monitoring discrepancies
    - SANDWICH method doesn't use OC measurements but instead gets OA through mass balance with PM2.5
    - Is there some OA in the OPM2.5 emissions
  - Missing SVOCs from inventory (VBS SOA module will address)
  - Higher underestimation in summer implies missing some SOA
- OPM2.5 overestimation tendency
  - Different monitoring artifacts in PM2.5 mass and speciated PM2.5 measurements make taking their difference problematic
  - Model OPM2.5 from emissions modeling speciation profiles
  - Given these uncertainties hard to interpret OPM2.5 performance

Ozone and PM Source Apportionment Modeling

- 2008 Base Case emissions scenario
- State-Specific Source Apportionment
  - Source Regions: Western States
  - Source Categories: Natural (Biogenic, Lightning, Sea Salt and WBD), Fire (separately for WF, Rx, AG) and Anthropogenic
  - CSAPR-type transport analysis
    - Examine upwind state anthropogenic (Anthro+Rx+Ag) contribution to downwind state ozone and $PM_{2.5}$ Design Values (DV)
    - CSAPR used "significance threshold" of 1% of NAAQS
  - Spatial extent of state contributions to high ozone/$PM_{2.5}$
    - For example, maximum state ozone contribution to daily maximum 8-hour ozone ≥ 76, 70, 65, 60 and 0 ppb

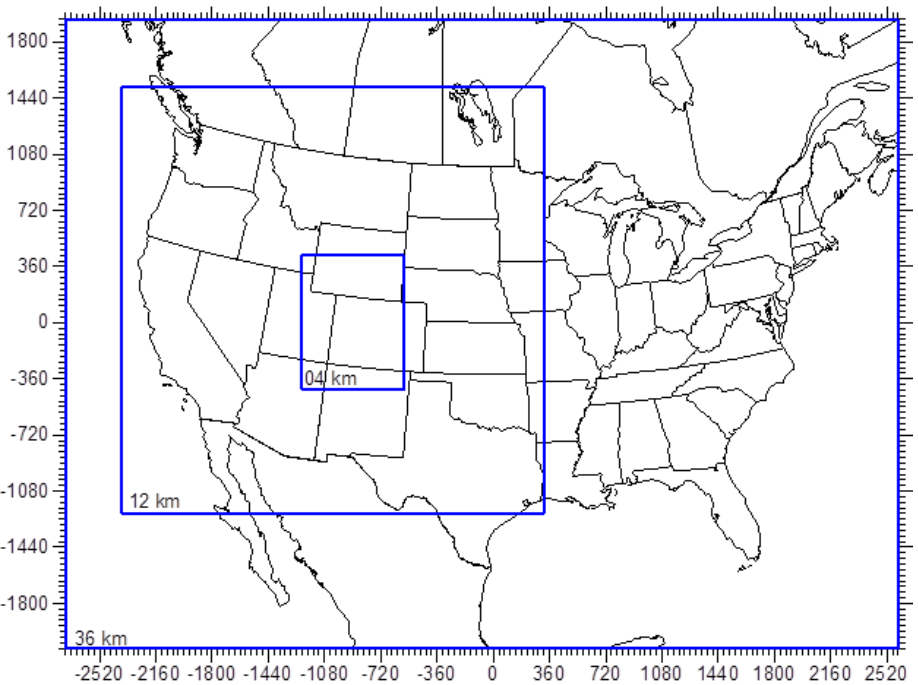
State-Specific Source Apportionment
21 Source Regions



Ozone and PM Source Apportionment Modeling

- Detailed Source Category-Specific Source Apportionment
  - Natural (Biogenic, lighting and sea salt)
  - Canada/Mexico
  - Fires (WF, Rx and Ag)
  - Upstream Oil and Gas (All – 2008 WRAP Phase III plus NEI)
  - Point Sources (EGU and non-EGU)
  - Mobile Sources (On-Road + Non-Road + CMV)
  - Remainder (Area, Ag Ammonia, FD, etc.)
- Current Status
  - State-Specific 2008 36/12 km Ozone – Done
  - State-Specific 2008 36 km PM – Running
  - Detailed Source Category-Specific 2008 36/12/4 km Ozone – to do
  - Detailed Source Category –Specific 2008 36/12 km PM – to do

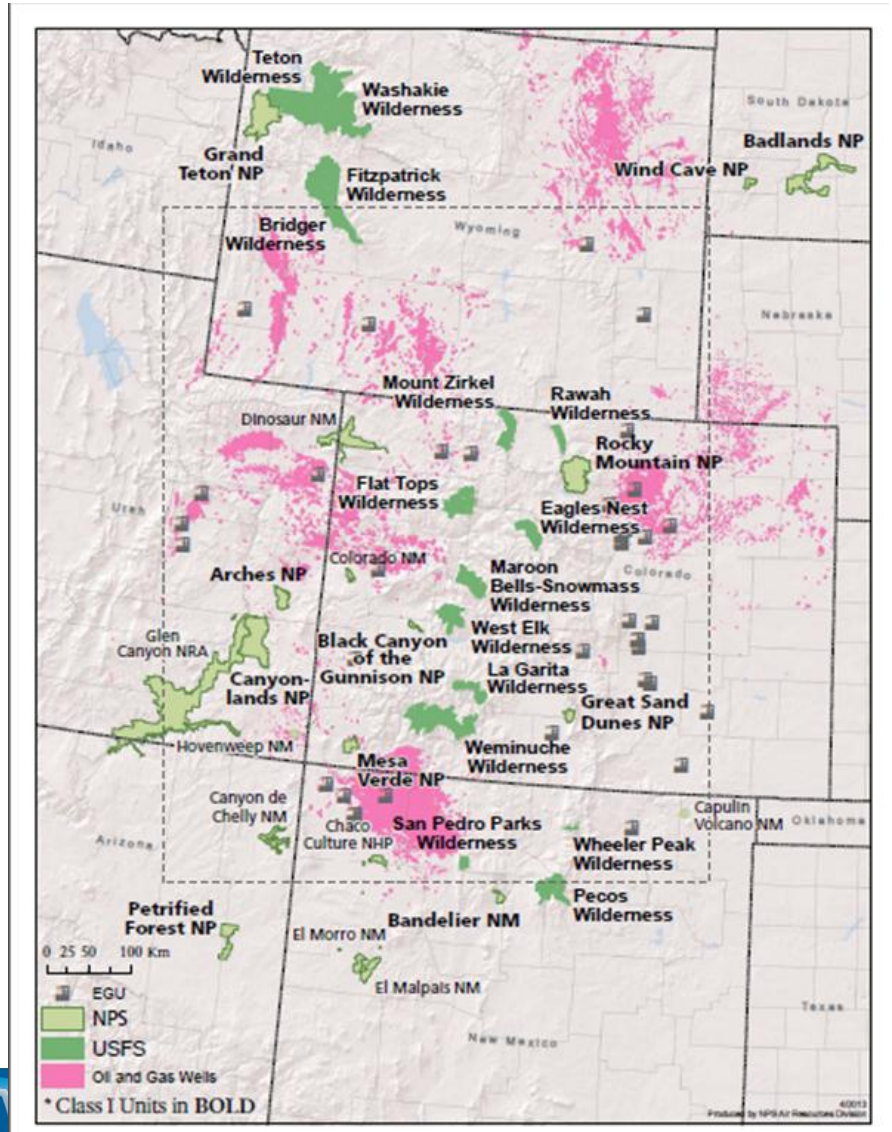
36/12/4 km Nests and 4 km DSAD



CAMx Modeling Domain

36 km : 148 x 112 (-2736, -2088) to (2592, 1944)
12 km*: 227 x 230 (-2388, -1236) to (336, 1524)
04 km*: 164 x 218 (-1228, -436) to (-572, 436)

* includes buffer cells



CSAPR-type Analysis

- State-Specific Anthropogenic (Anthro+Rx+Ag) contributions to 8-hour ozone Design Value (DVs)
- Model Attainment Test Software (MATS) to project current DVs without a selected state's contribution
  - Use relative change in model results to scale observed current year DV (DVC) in absence of a state's anthropogenic emissions
  - Difference is state's ozone contribution at each ozone monitoring site
- As in CSAPR, use two sets of DVCs
  - AvgDVC = Average of 2006-2008, 2007-2009 & 2008-2010 DVs
  - MaxDVC = Maximum of 2006-08, 2007-09 & 2008-10 DVs
- CSAPR used significant contribution threshold of 1% of the NAAQS

2008 36/12 km State-Specific Analysis

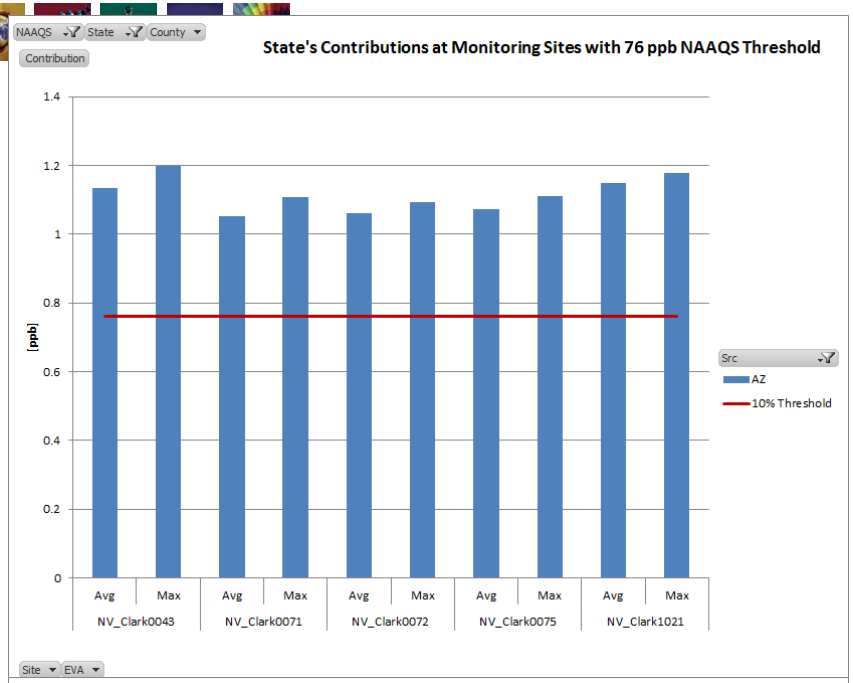
- CSAPR-type Analysis using current (March 2008) 0.075 ppm ozone NAAQS
  - Also looking at 70, 65 and 60 ppb future NAAQS
- 136 ozone monitors in 12 km WESTUS domain with AvgDVC exceeding NAAQS (76 ppb or higher) [86/63% in CA and
- Maximum (ppb) and number of downwind state monitors with upwind state ozone contribution above 1 % of NAAQS (0.76 ppb):

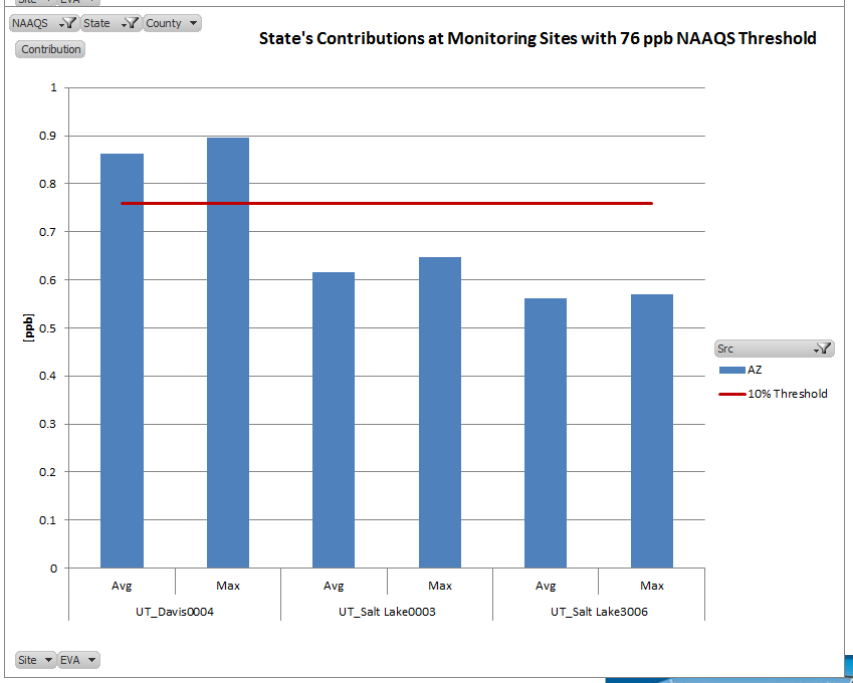
Maximum	**1.23**	**16.65**	0.51	**8.95**	**1.02**	0.39	**6.52**	**1.13**	**1.03**
Count	24	18	0	4	2	0	18	25	1
Source State	AZ	CA	CO	KS	ID	MT	OK	OR	WA

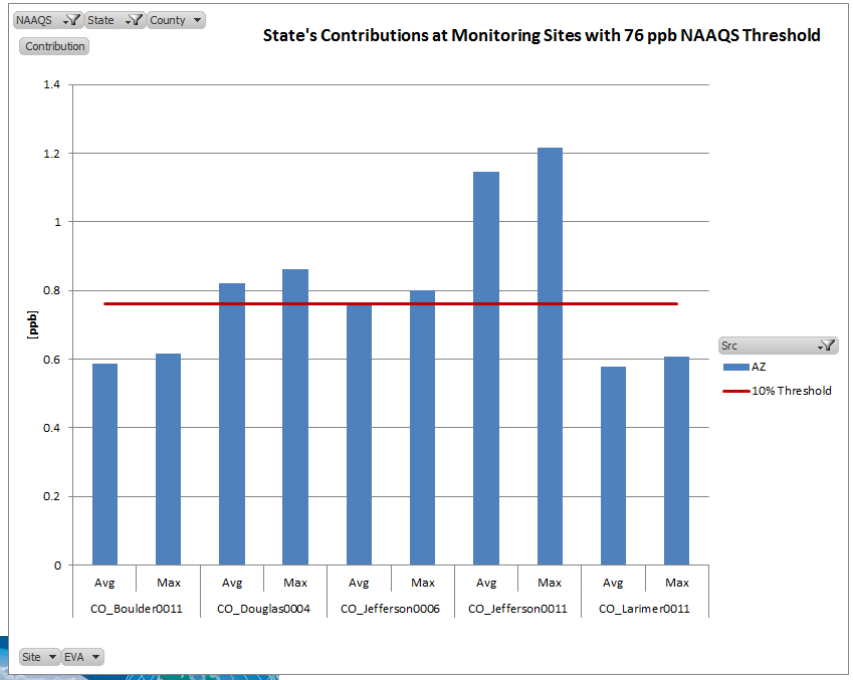
Maximum	**1.53**	0.12	0.13	0.36	**1.28**	**2.53**	**10.17**	**0.82**
Count	5	0	0	0	20	5	6	2
Source State	WY	ND	SD	NE	NV	UT	TX	NM

ENVIRON

Arizona Contributions to AvgDVC ≥ 76 ppb (13 sites in CA) NV, UT and CO

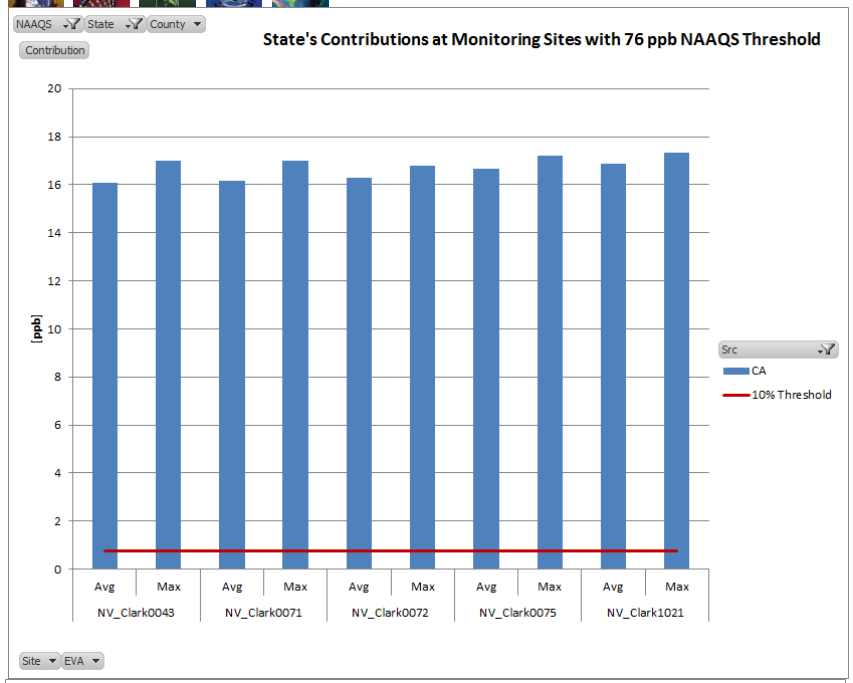


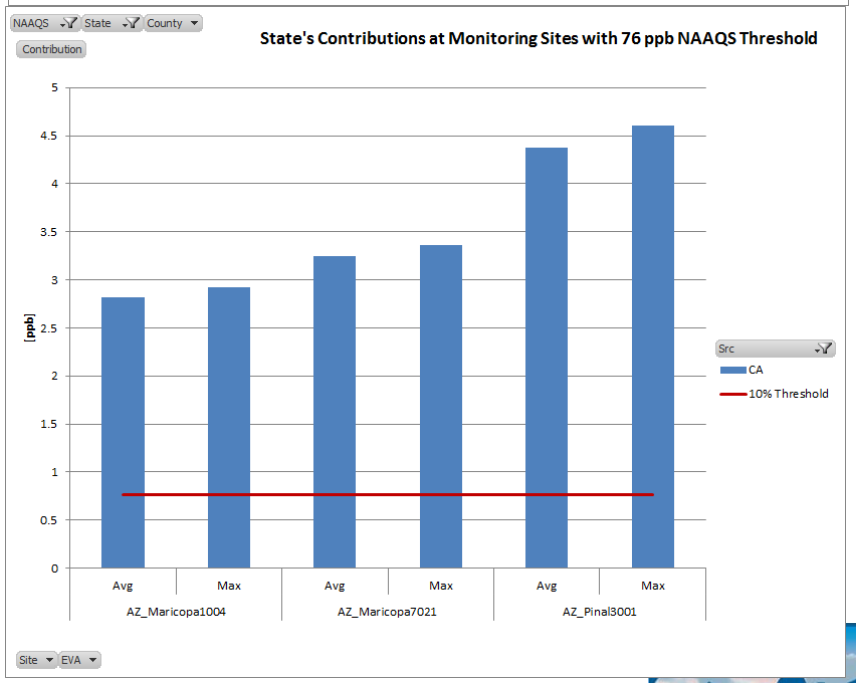


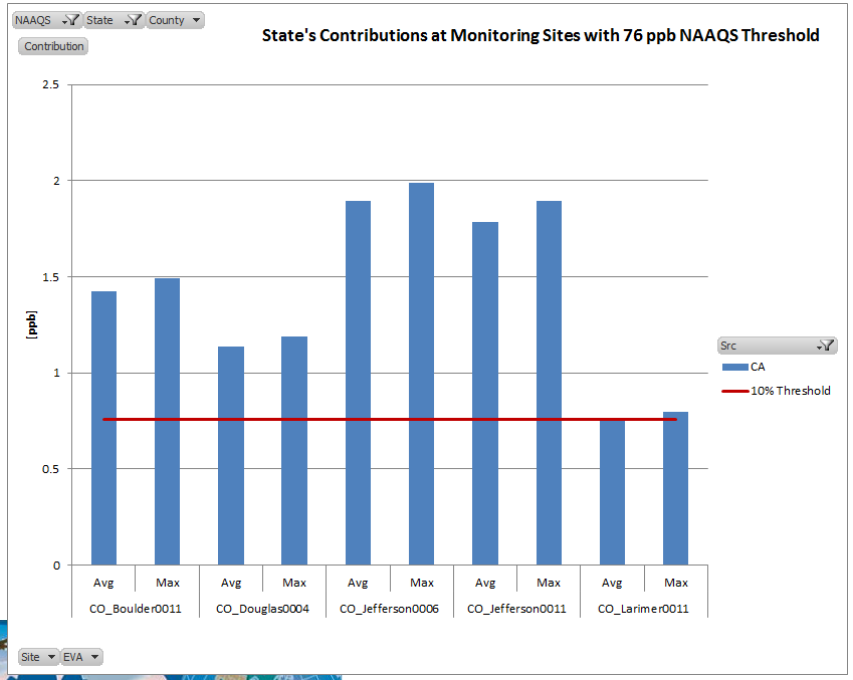


WESTERN REGIONAL AIR PARTNERSHIP

California contribution to NV, AZ and CO



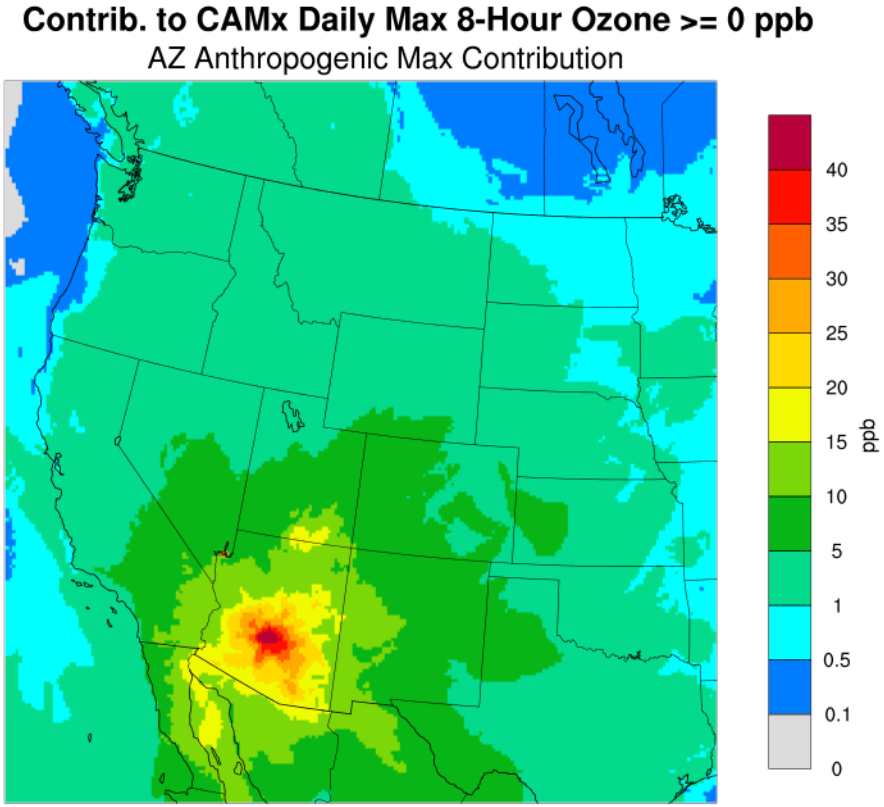


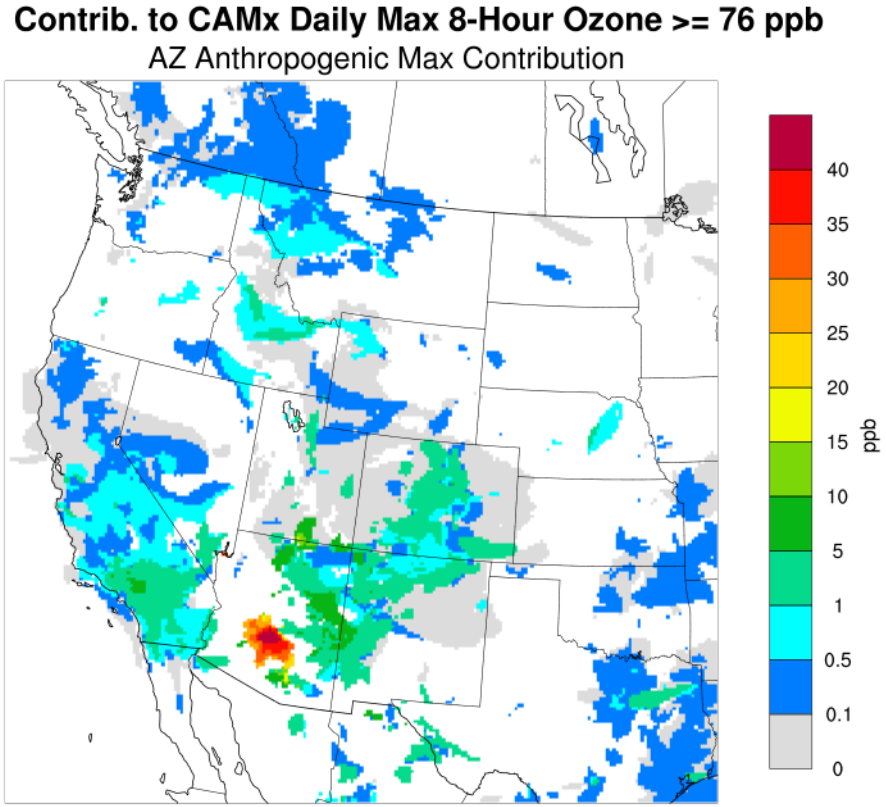


State-Specific Ozone Foot Prints

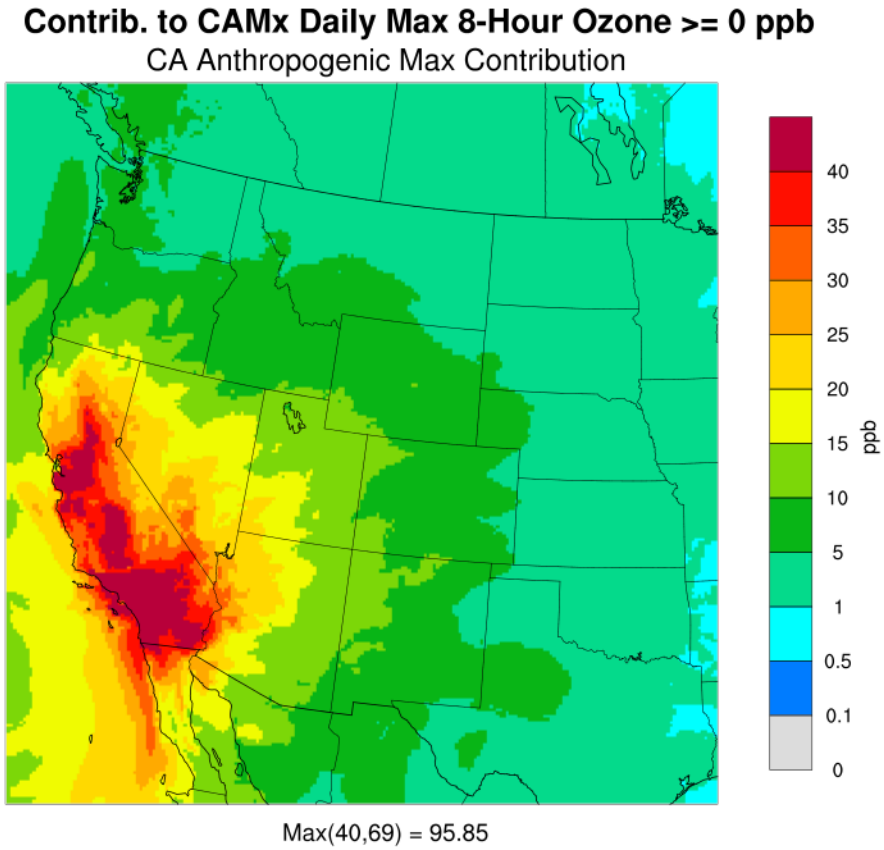
- Examine spatial distribution of state's highest contribution to modeled daily maximum 8-hour ozone concentrations for total modeled ozone greater than or equal to several thresholds:
  - 76 ppb (current NAAQS)
  - 70 ppb
  - 65 ppb
  - 60 ppb
  - 0 ppb (highest contribution in year)
- Results follow for 0 ppb and 76 ppb

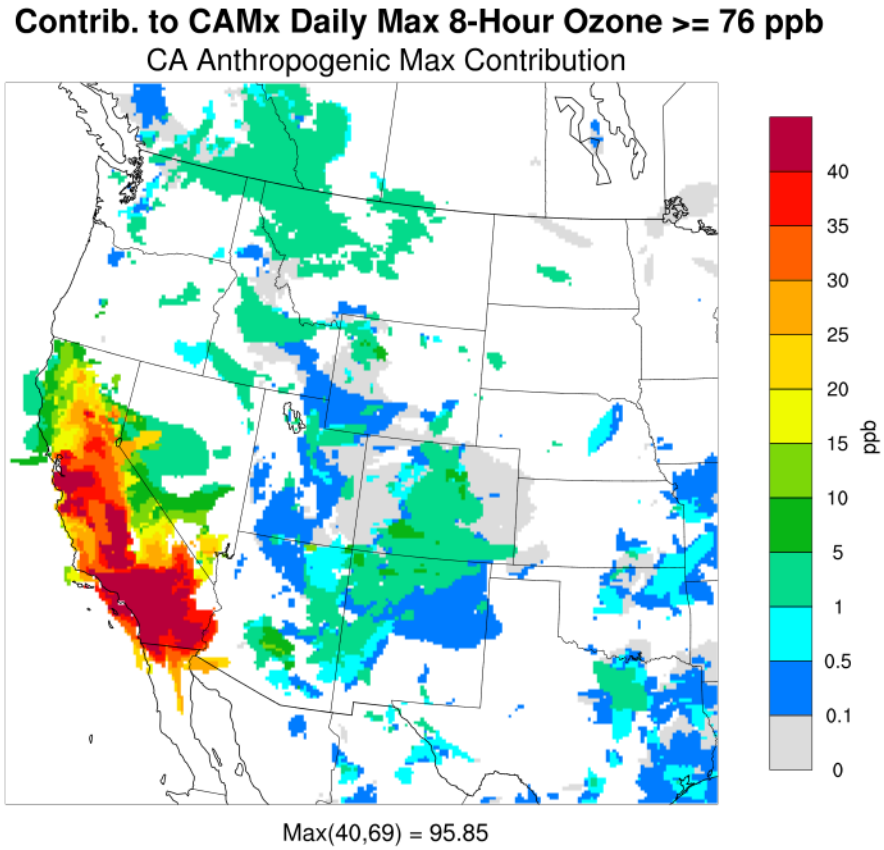
Arizona Highest 8-Hour Ozone Contribution



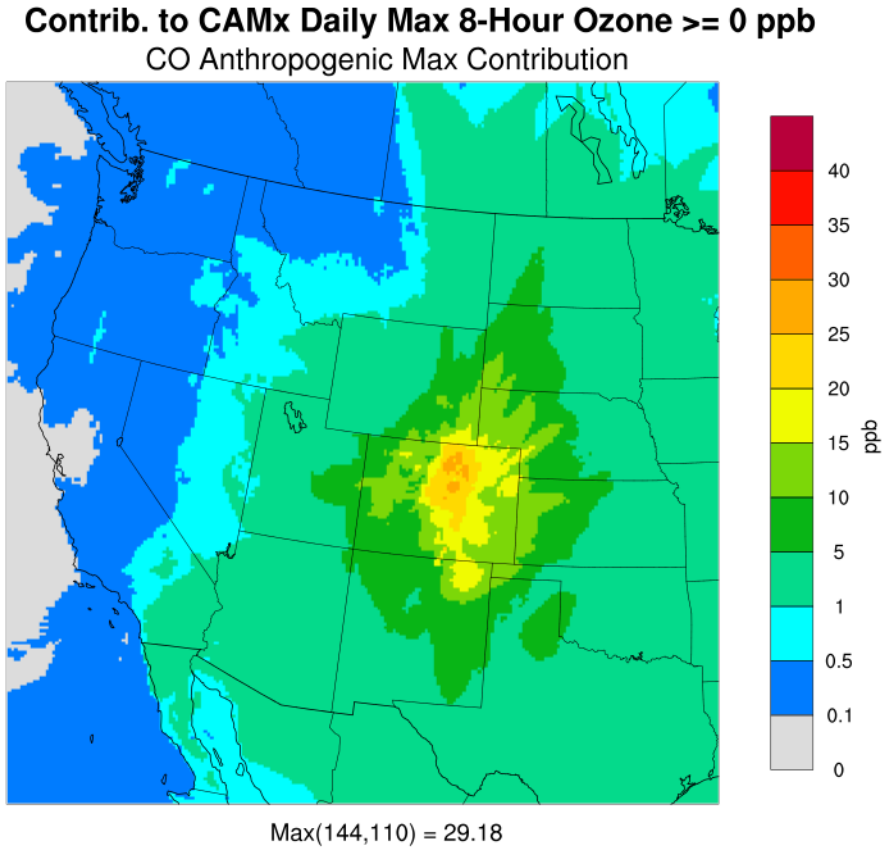


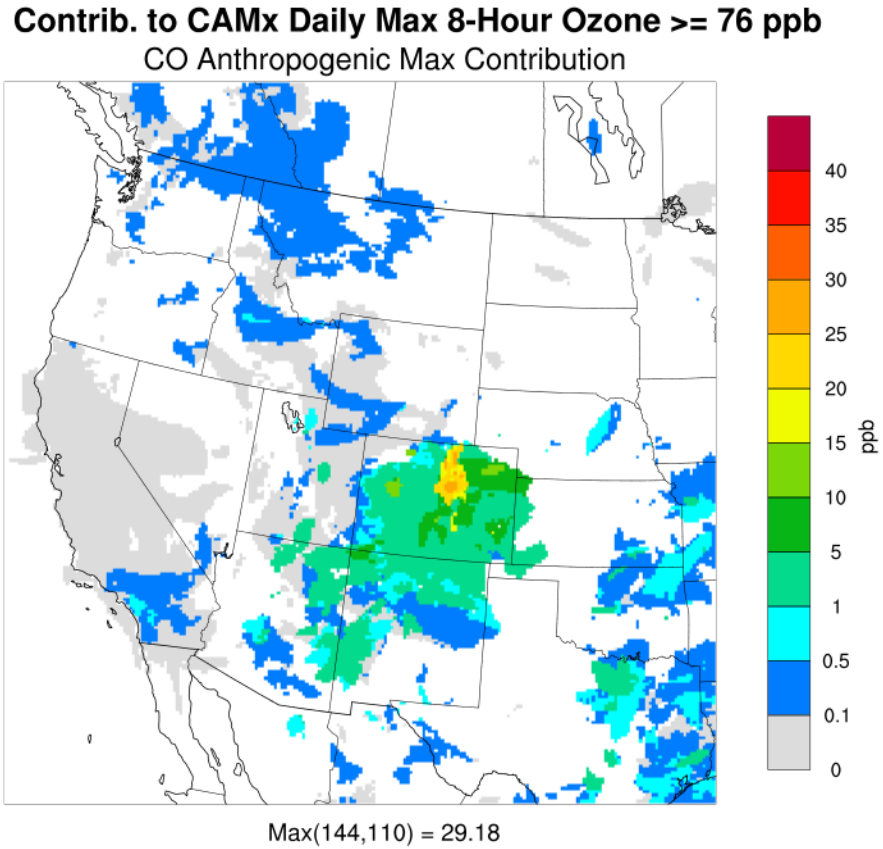
California Highest 8-Hour Ozone Contribution



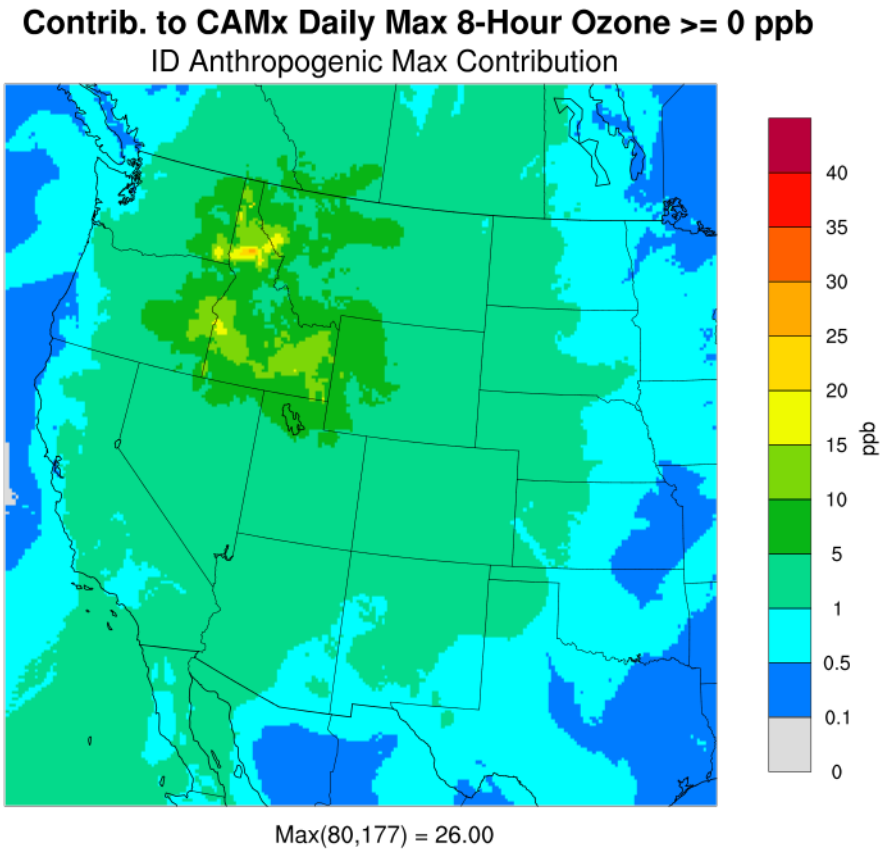


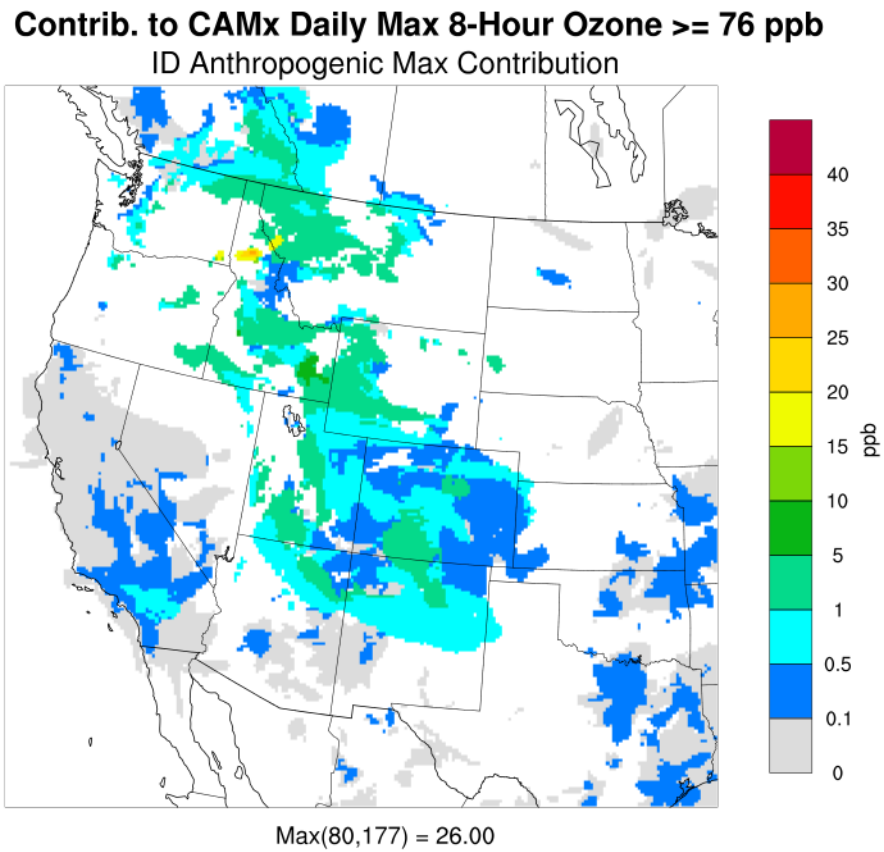
Colorado Highest 8-Hour Ozone Contribution



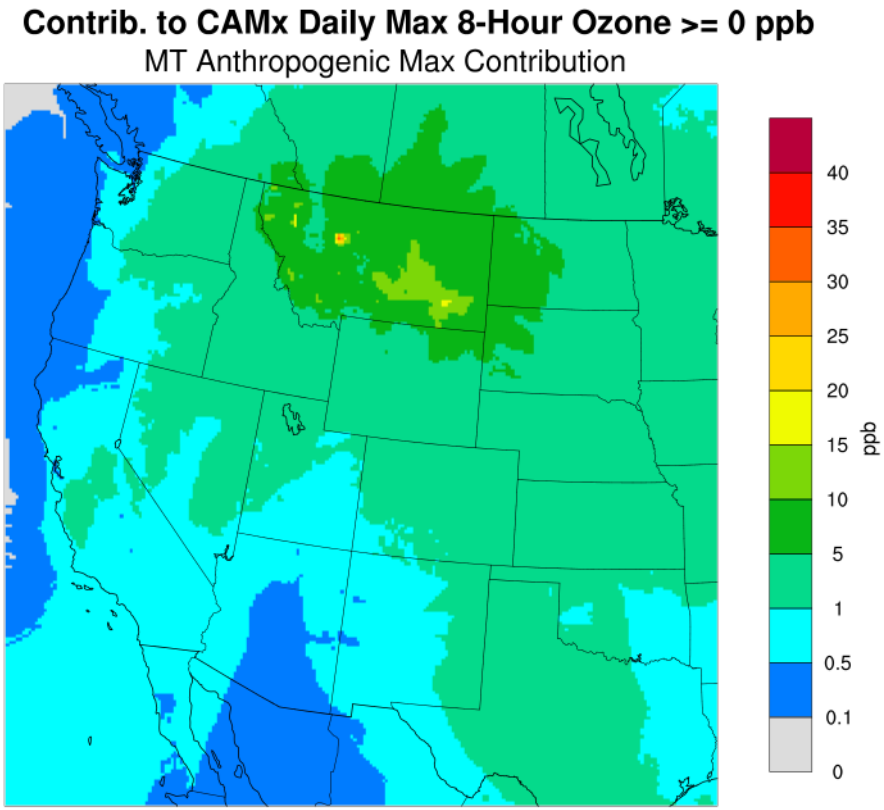


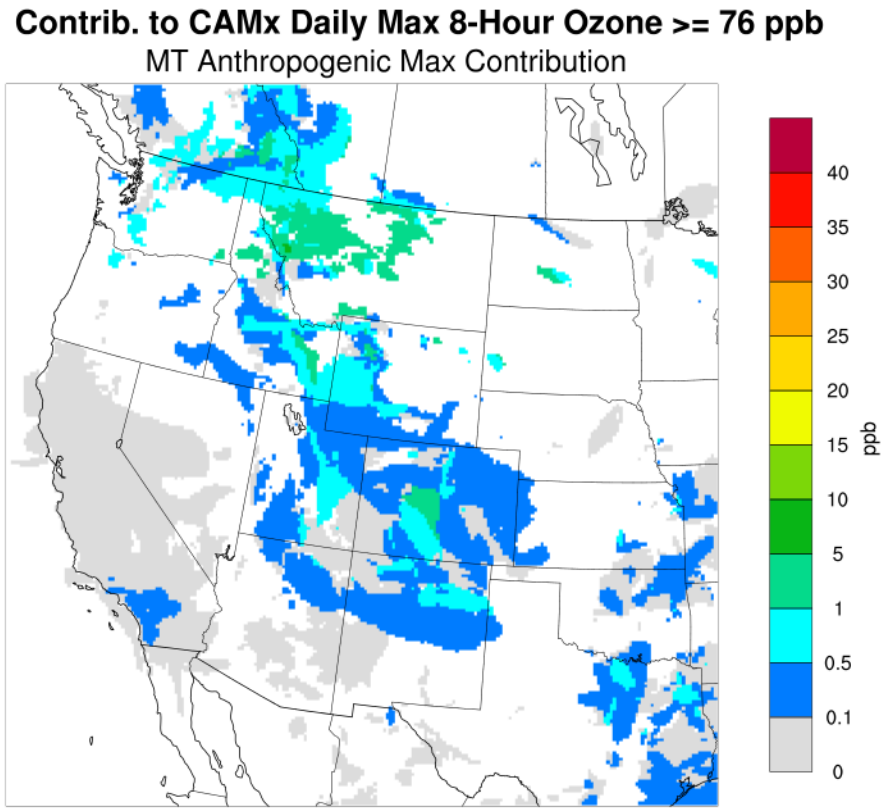
Idaho Highest 8-Hour Ozone Contribution



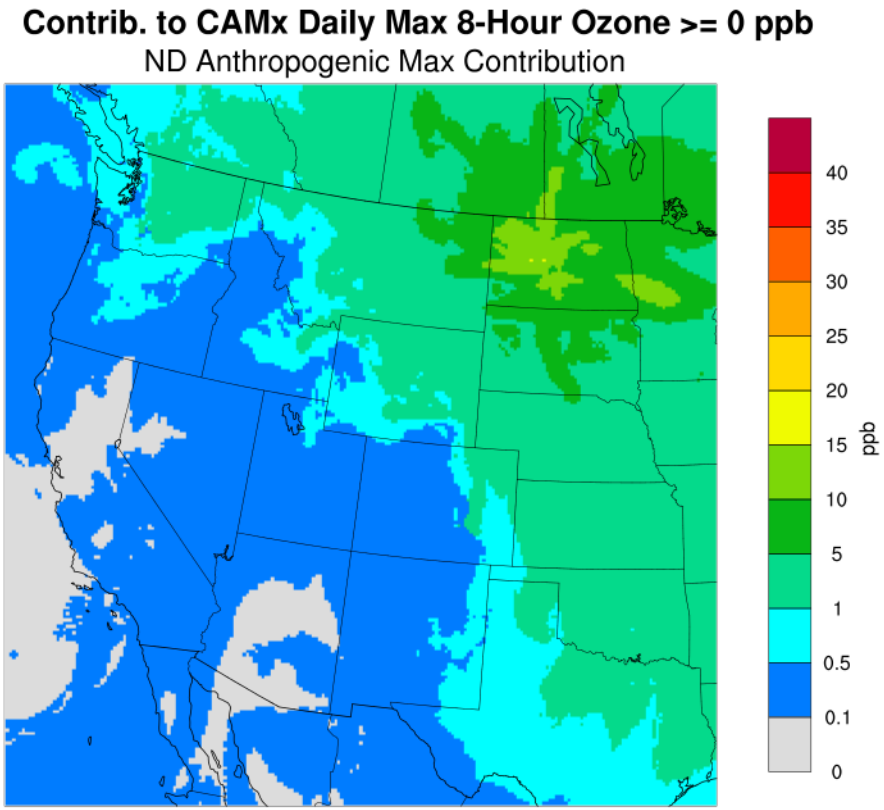


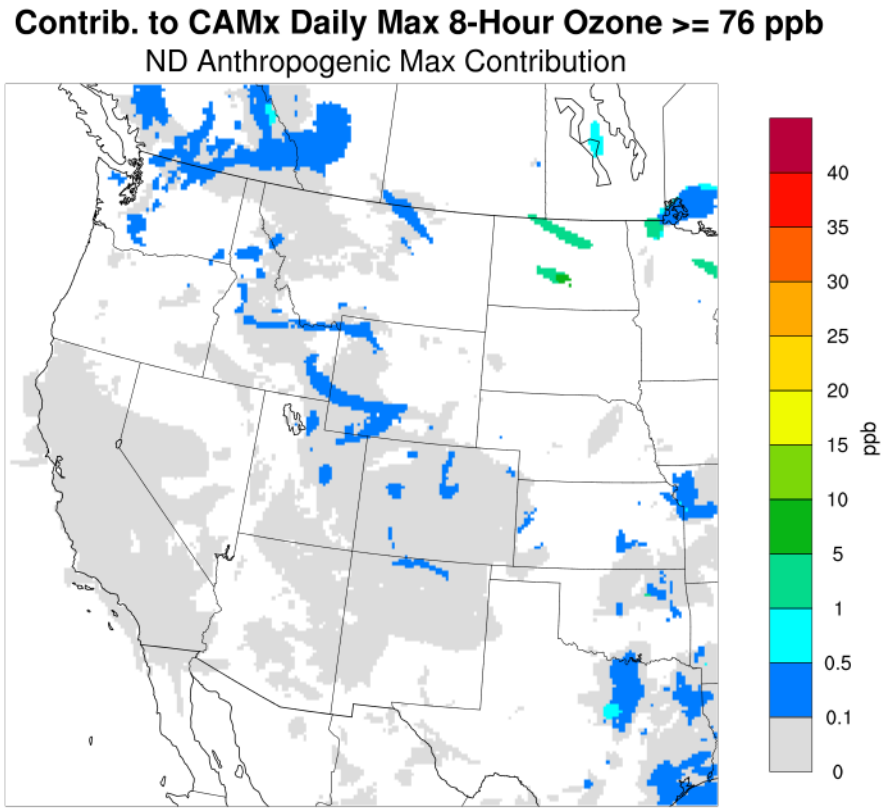
Montana Highest 8-Hour Ozone Contribution



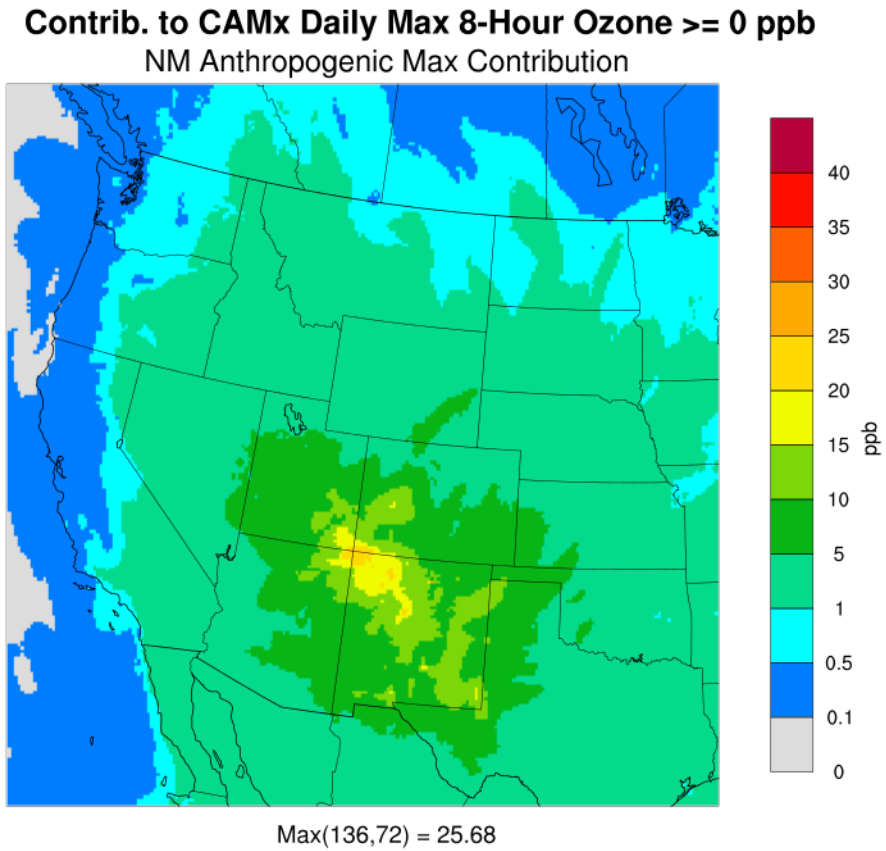


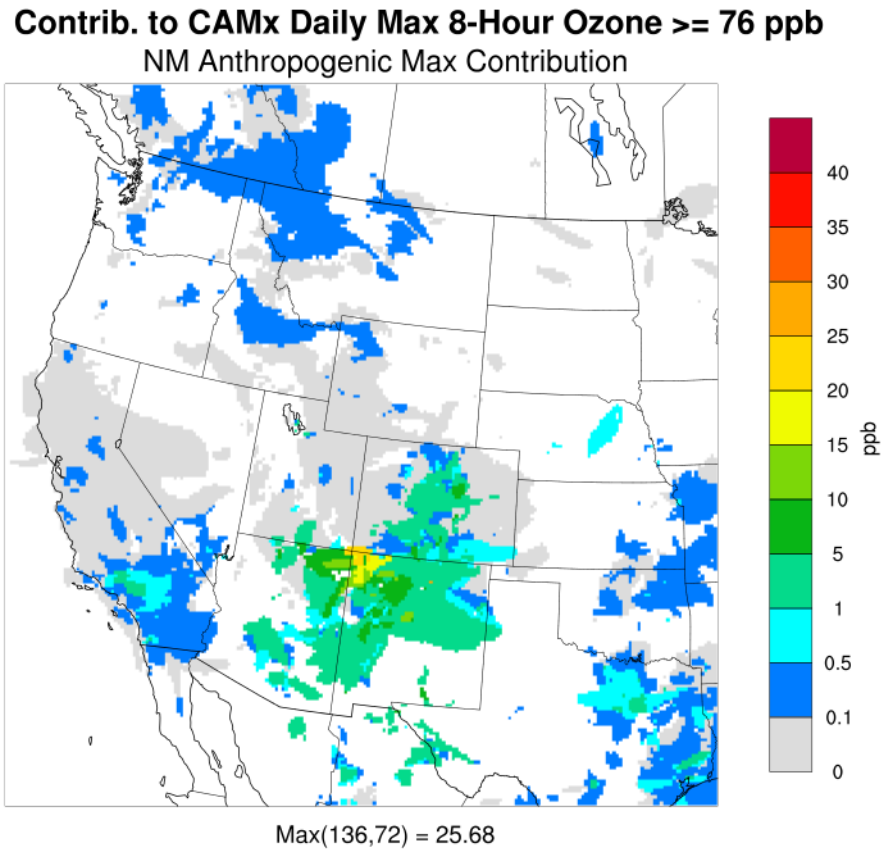
North Dakota Highest 8-Hour Ozone Contribution



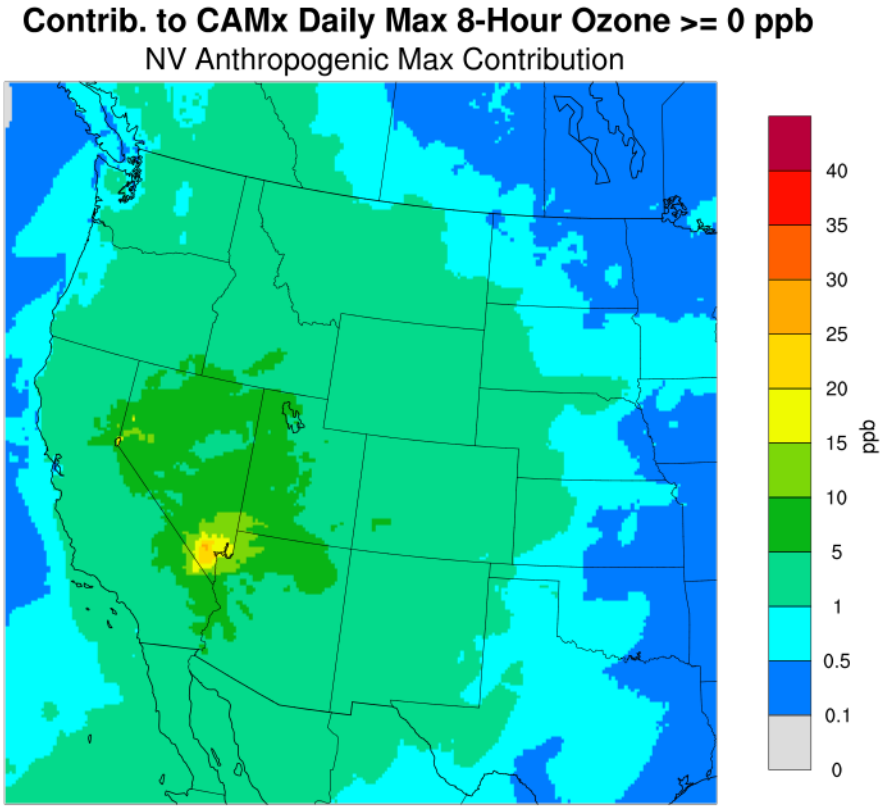


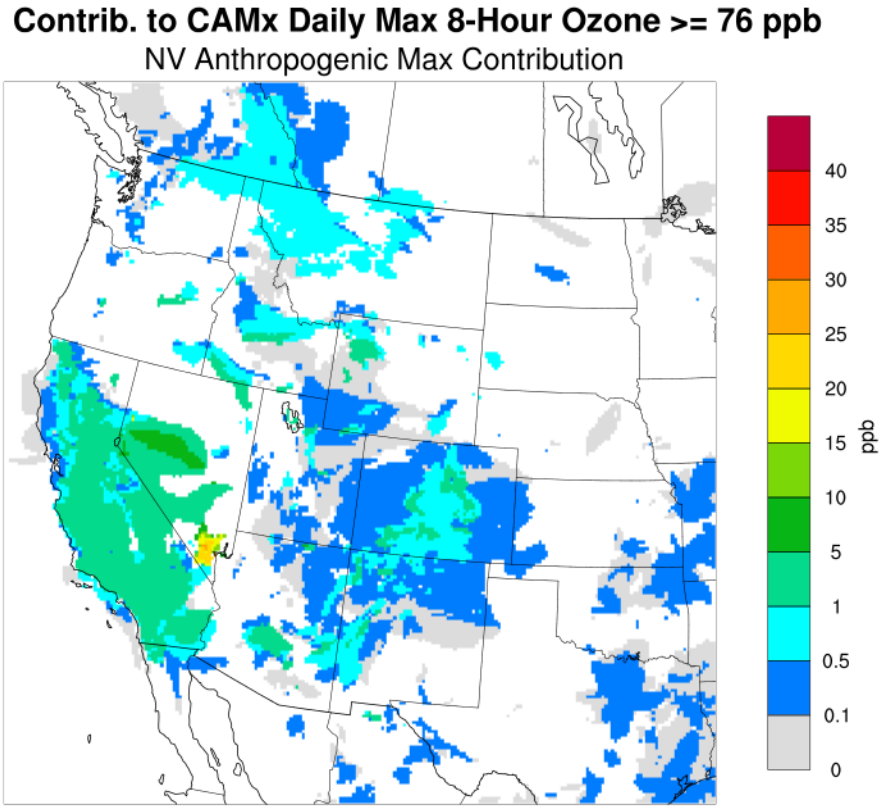
New Mexico Highest 8-Hour Ozone Contribution



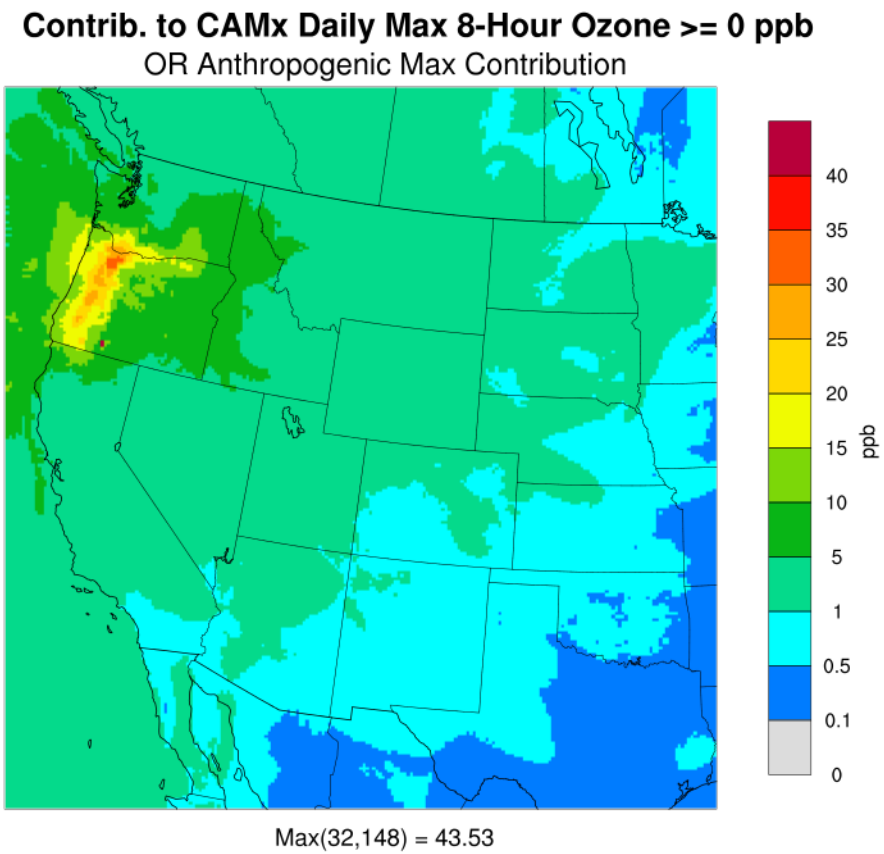


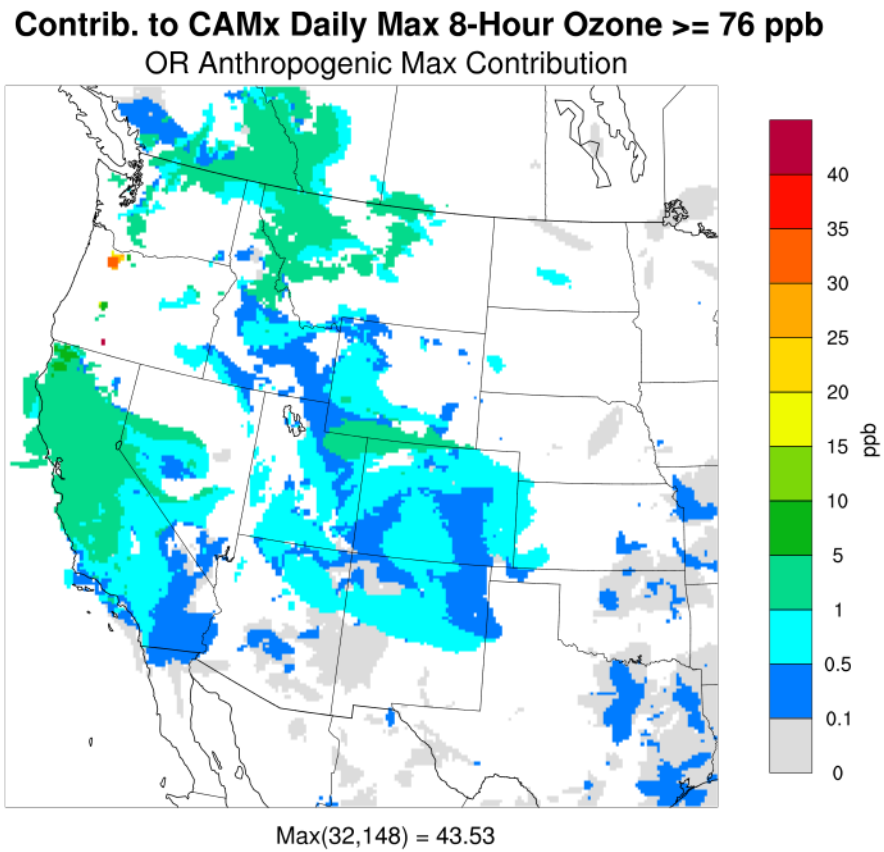
Nevada Highest 8-Hour Ozone Contribution



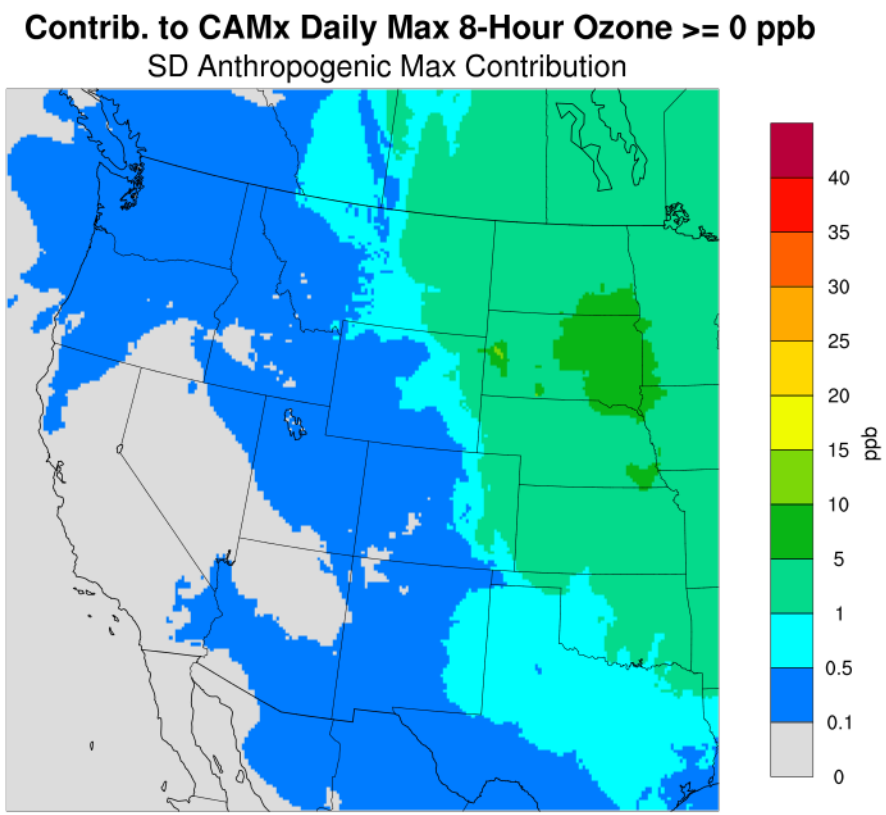


Oregon Highest 8-Hour Ozone Contribution

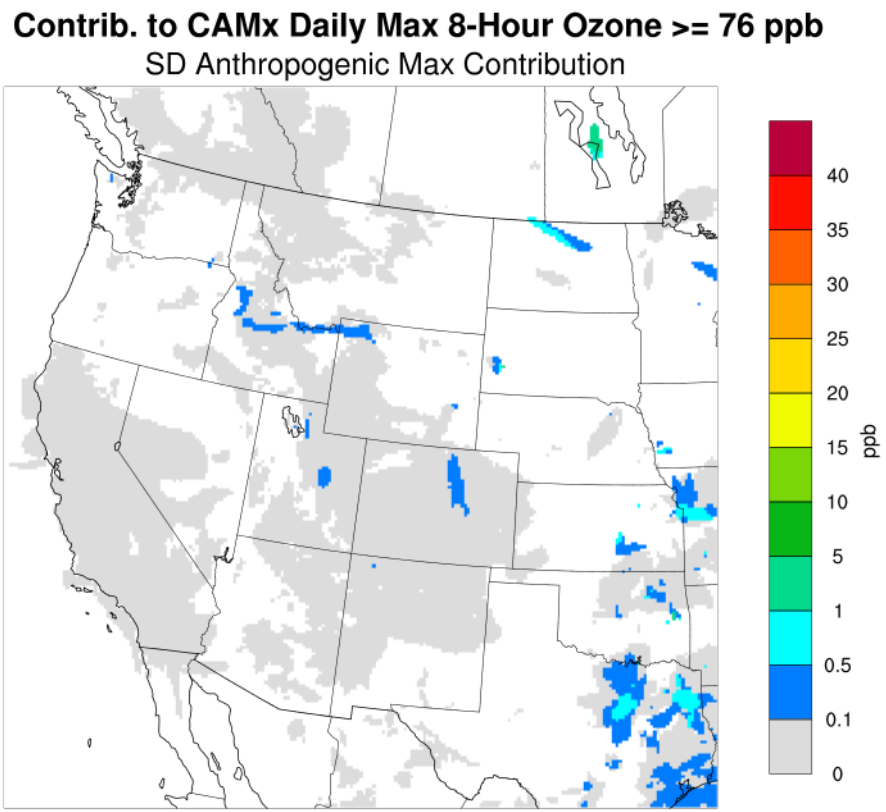




South Dakota Highest 8-Hour Ozone Contribution

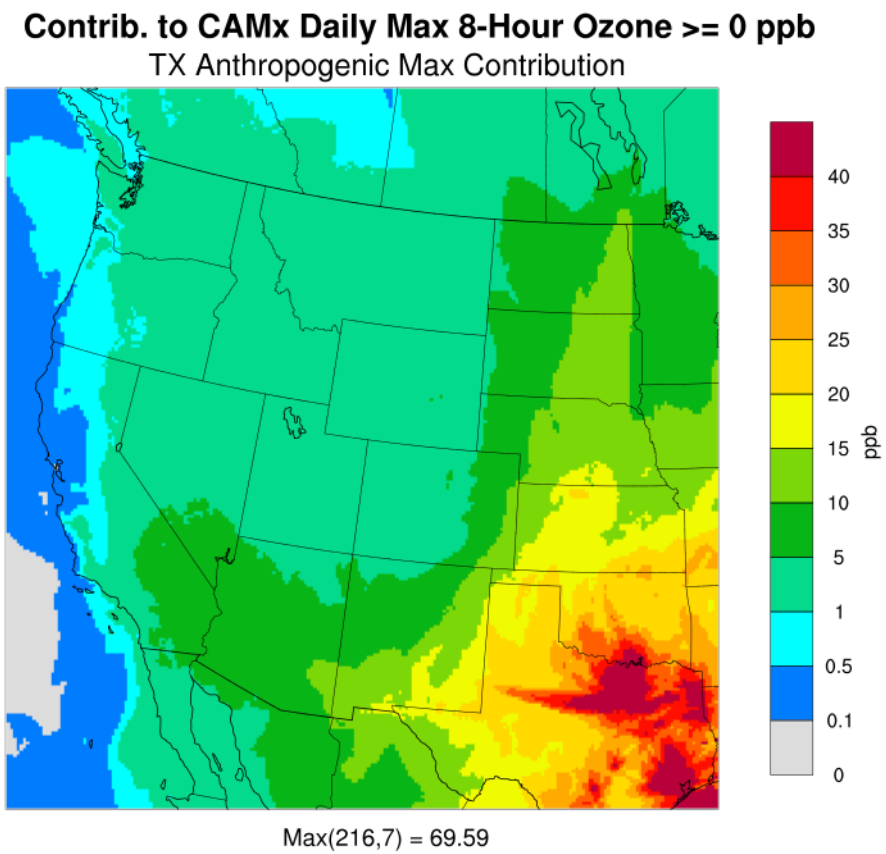


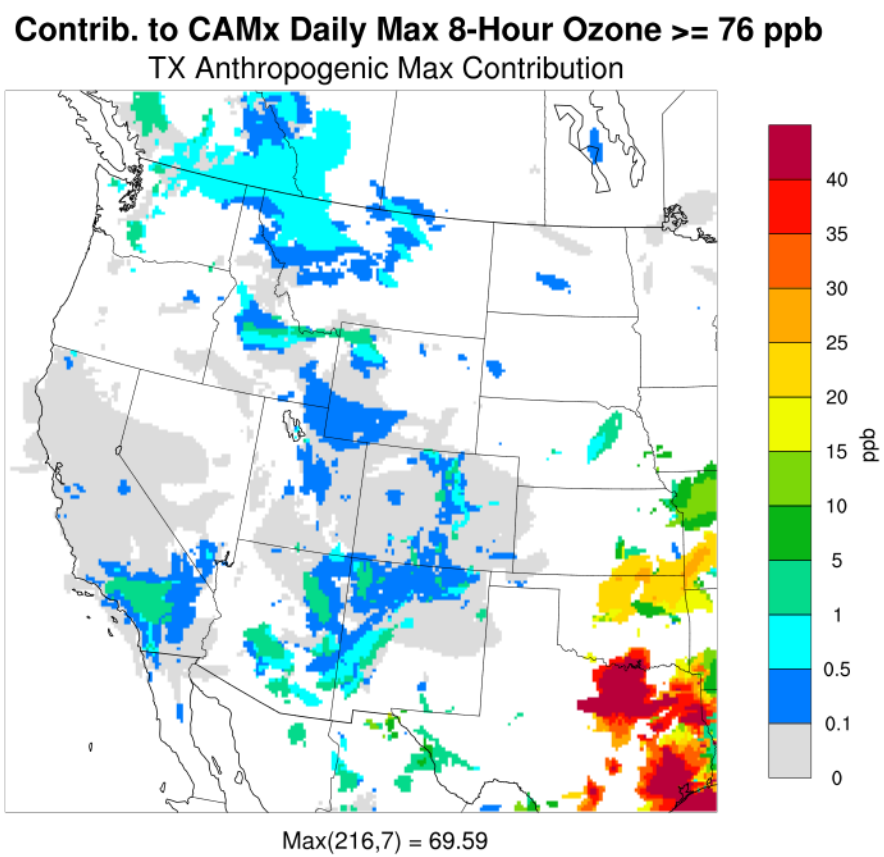
Max(157,146) = 12.72



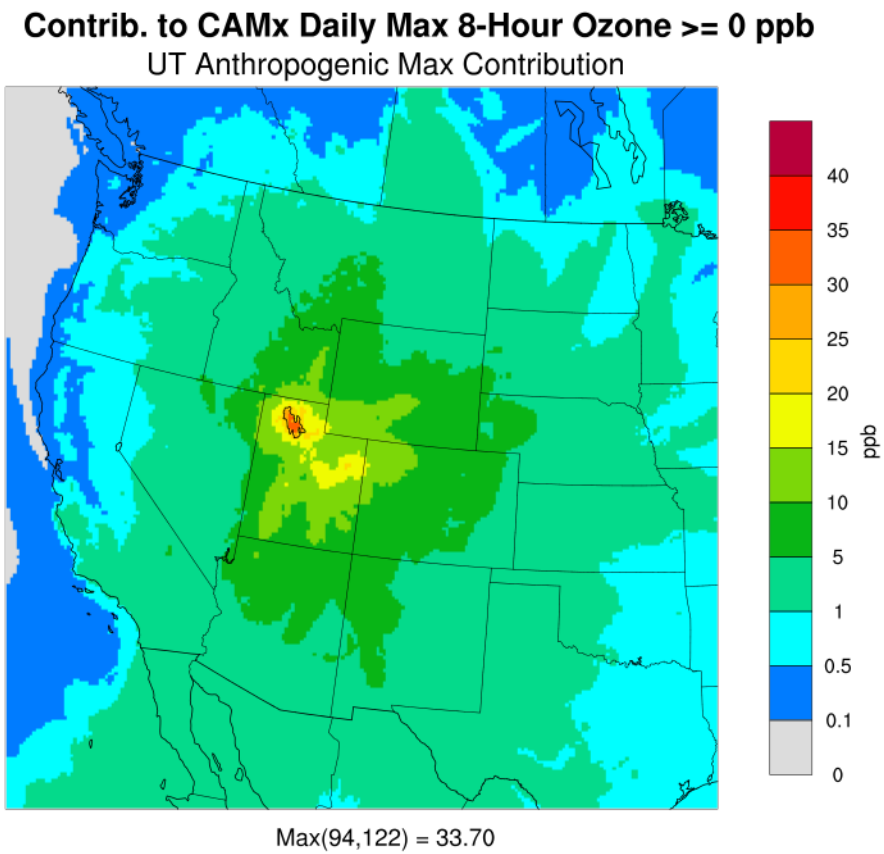
Max(159,141) = 1.46

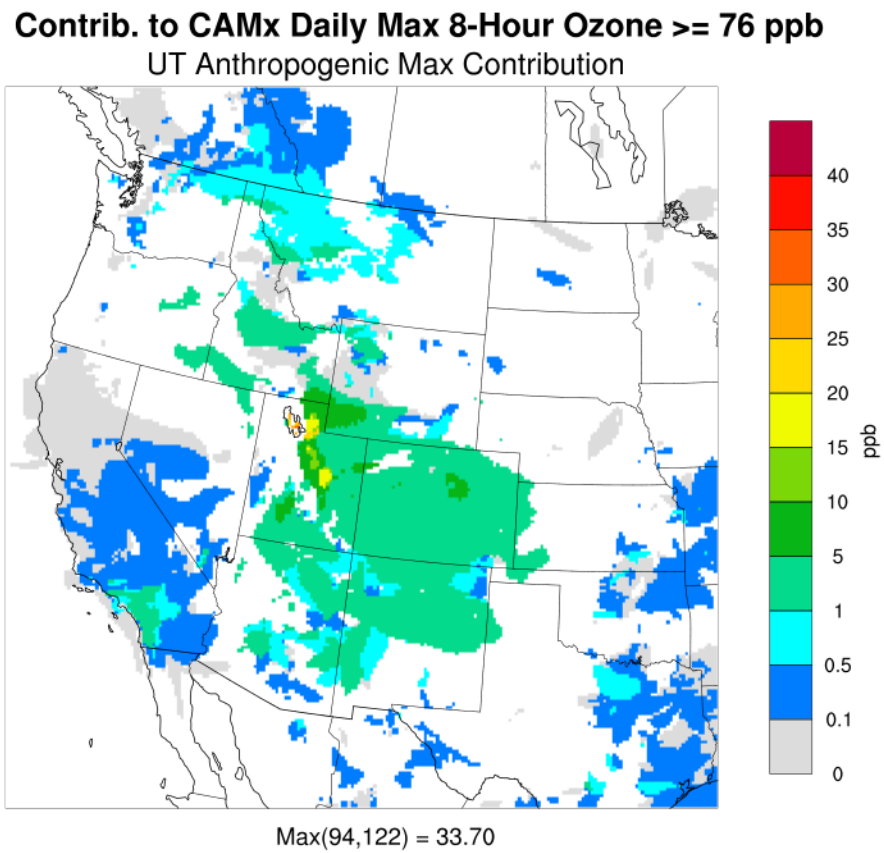
Texas Highest 8-Hour Ozone Contribution



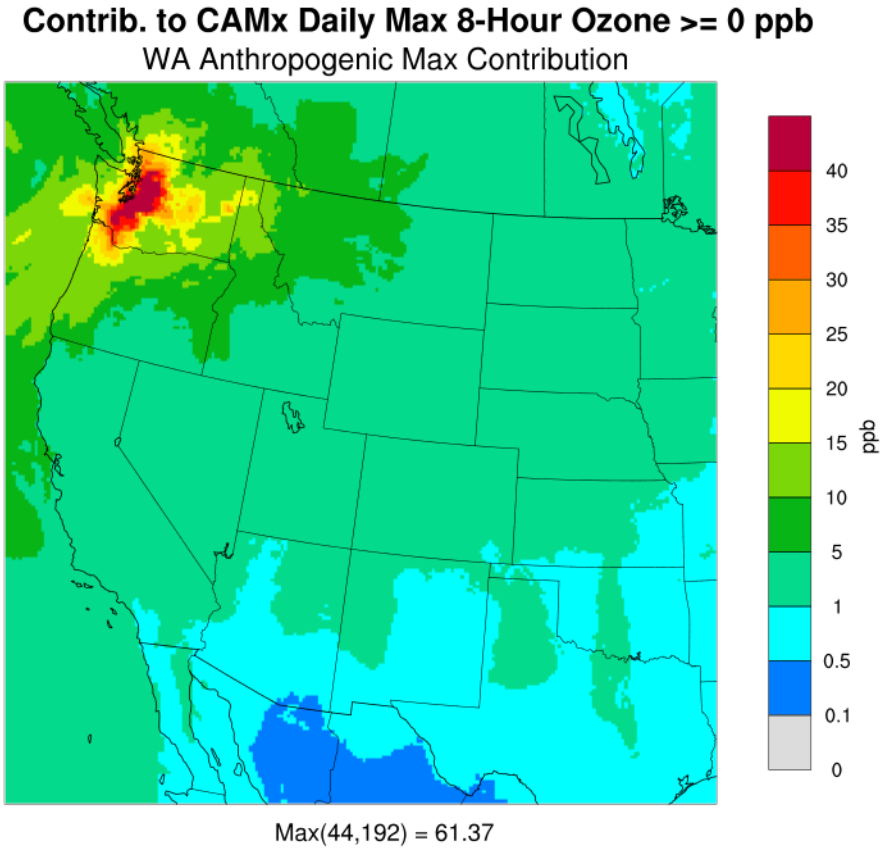


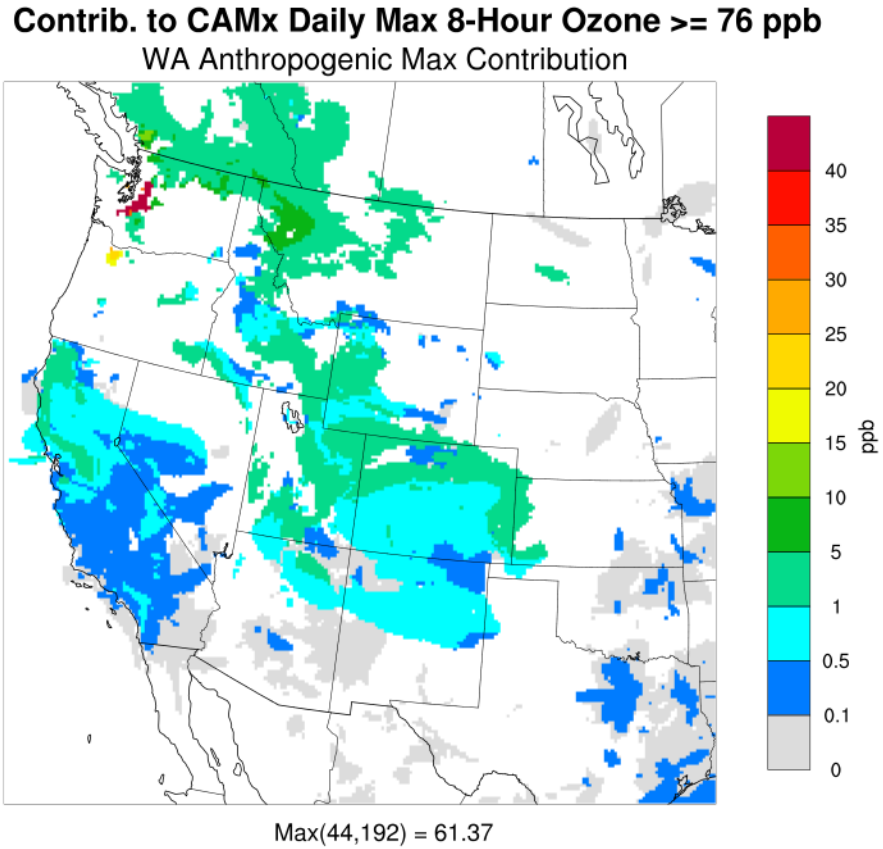
Utah Highest 8-Hour Ozone Contribution



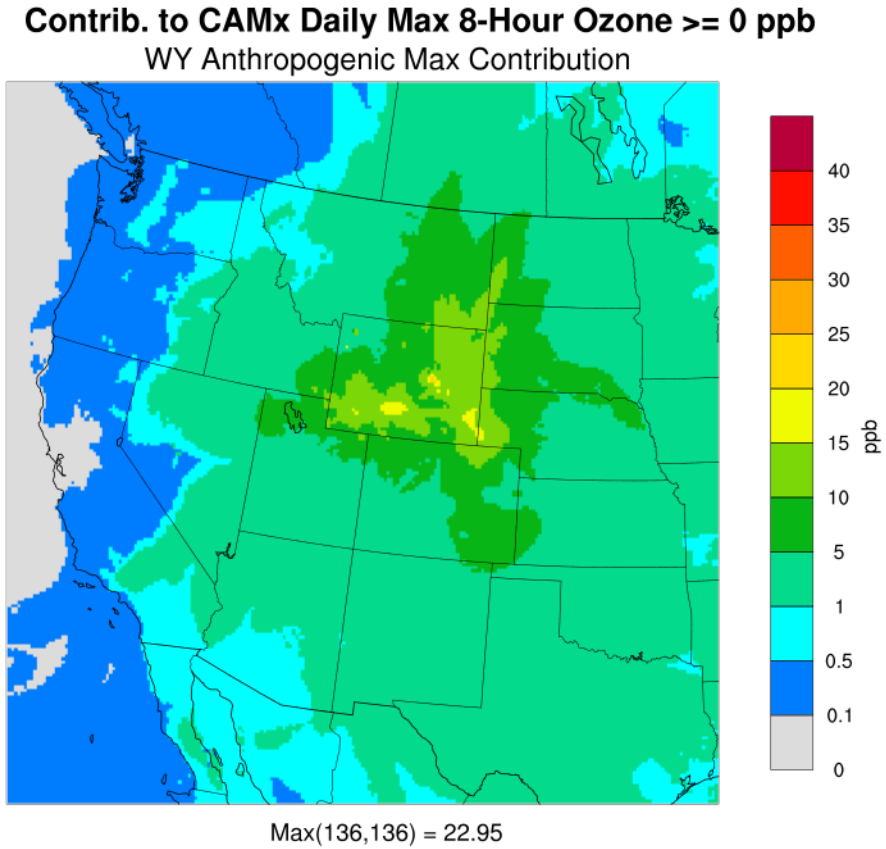


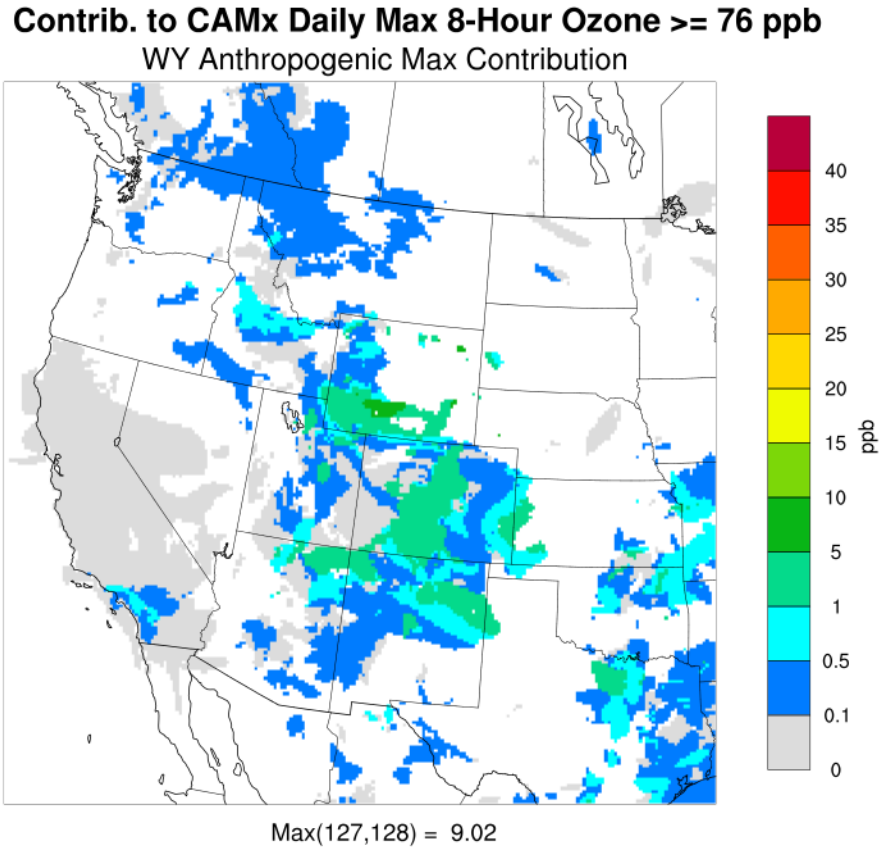
Washington Highest 8-Hour Ozone Contribution





Wyoming Highest 8-Hour Ozone Contribution





WestJumpAQMS Next Steps

- Complete State-Specific PM Source Apportionment Modeling
  - Displays of annual and 24-hour PM2.5
  - Visibility and Sulfur/Nitrogen Deposition
- Set up and start Source Category-Specific Ozone and PM Source Apportionment Modeling
- Next Conference Call July 17 @ 10am MDT
  - State-Specific PM Source Apportionment
  - Final Report Outline and Other