Predicting Ozone in the Colorado Front Range using EPA's Air Quality Model

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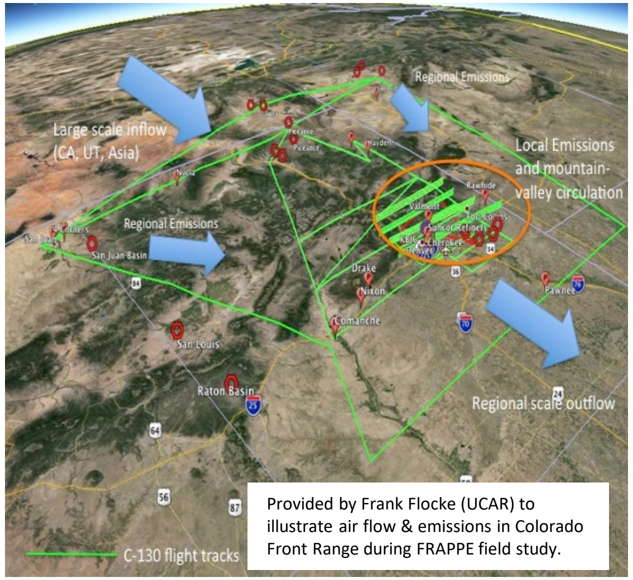
OVERVIEW:

- **Motivation:**
  - Denver Metro/North Front Range (DMNFR) ozone (O_3) nonattainment area (NAA) in Colorado has had unhealthy levels of ozone even though air quality programs have focused on reducing ozone precursor emissions.
  - It is speculated that effects of these emission reductions may be partially offset by increasing levels of background ozone and increases in local emissions from population growth and extensive oil and gas development in the area.
- **Objective:**
  - Develop a hemispheric-to-regional scale air quality model platform to simulate ozone transport and chemistry in the DMNFR NAA and to estimate source contributions to simulated ozone.



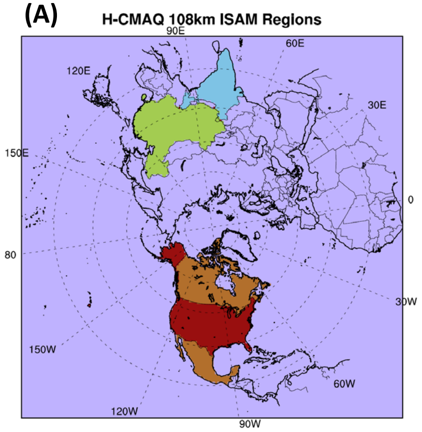
Provided by Frank Flocke (UCAR) to illustrate air flow & emissions in Colorado Front Range during FRAPPE field study.

- **Approach:**
  - Use the Weather Research and Forecasting (WRF) model, emissions from global datasets and the 2014 National Emissions Inventory (NEI), and the Hemispheric and Regional Community Multiscale Air Quality (H-CMAQ & CMAQ) model that includes the Integrated Source Apportionment Method (ISAM).
  - Assess model performance through a comprehensive evaluation and detailed comparisons with measurements of meteorological variables, ozone, and ozone precursor species from a variety of surface and airborne platforms.
  - Focus on July and August 2014 to align with the Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) and Front Range Air Pollution and Photochemistry Experiment (FRAPPE) field studies in Colorado.

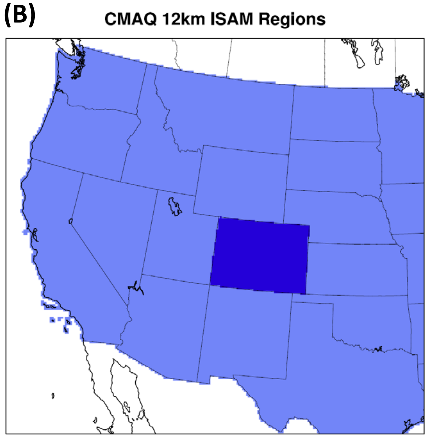
DESCRIPTION OF AIR QUALITY MODEL SET-UP:

Configuration	108-km Platform	12-km Platform	4-km Platform
Analysis Period	1/1/2014 – 12/13/2014	7/27/2014 – 8/16/2014	7/27/2014 – 8/16/2014
Simulation Period	10/1/2013 – 12/31/2014	7/1/2014 – 8/31/2014	7/1/2014 – 8/31/2014
Meteorology	WRF v4.0.2	WRF v3.8.1	WRF v3.8.1
CMAQ Version	CMAQv5.3.2 with ISAM	CMAQv5.3.2 with ISAM	CMAQv5.3.2 with ISAM
CMAQ Options	cb6r3m, aero7, m3dry dry deposition, no bi-directional NH3	cb6r3, aero7, m3dry dry deposition, bi-directional NH3	cb6r3, aero7, m3dry dry deposition, bi-directional NH3
Vertical Layers	44	35	35
Anthropogenic Emissions	2016 H-CMAQ modeling platform	2014 NEIv2 modeling platform	2014 NEIv2 modeling platform
Biogenic Emissions	GEIA climatology	BEIS Inline	BEIS Inline
Fires	FINN	2014 NEIv2	2014 NEIv2
Lightning NO Emissions	GEIA climatology	Inline	Inline
Windblown Dust Emissions	Inline	None	None
ISAM Configuration	16 Tags (5 source regions, 5 emission sectors, stratosphere, initial/boundary conditions, other)	13 Tags (2 source regions, 5 emission sectors, initial/boundary conditions, other)	18 Tags (3 source regions, 5 emission sectors, initial/boundary conditions, other)
Model Domain & ISAM Source Regions	See Figure A	See Figure B	See Figure C

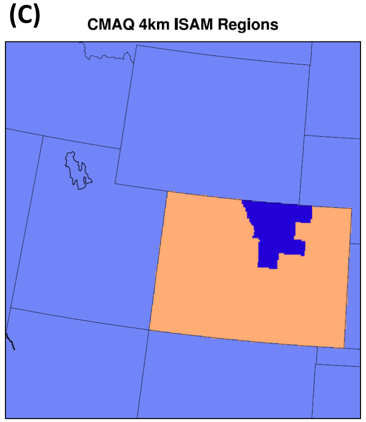
(A)



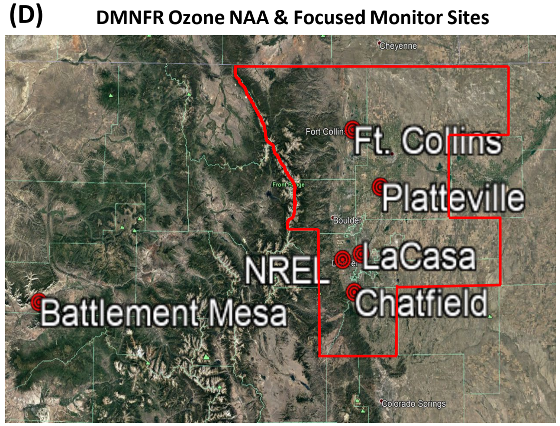
(B)



(C)



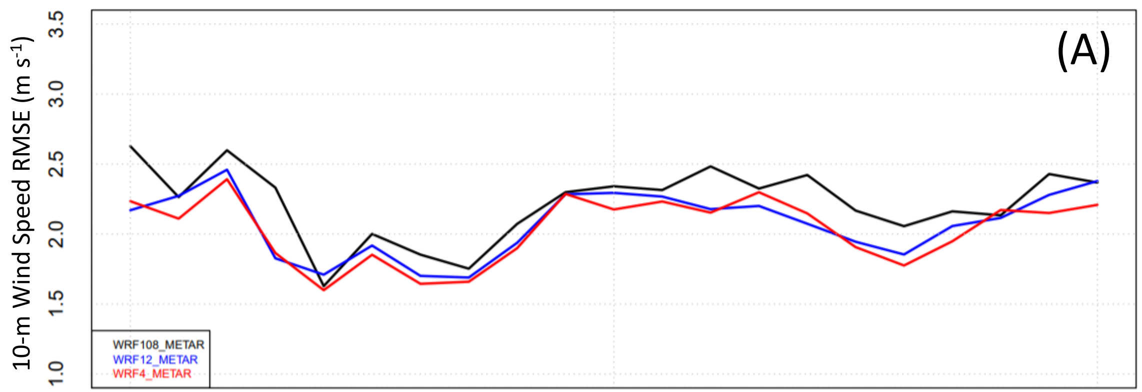
(D)

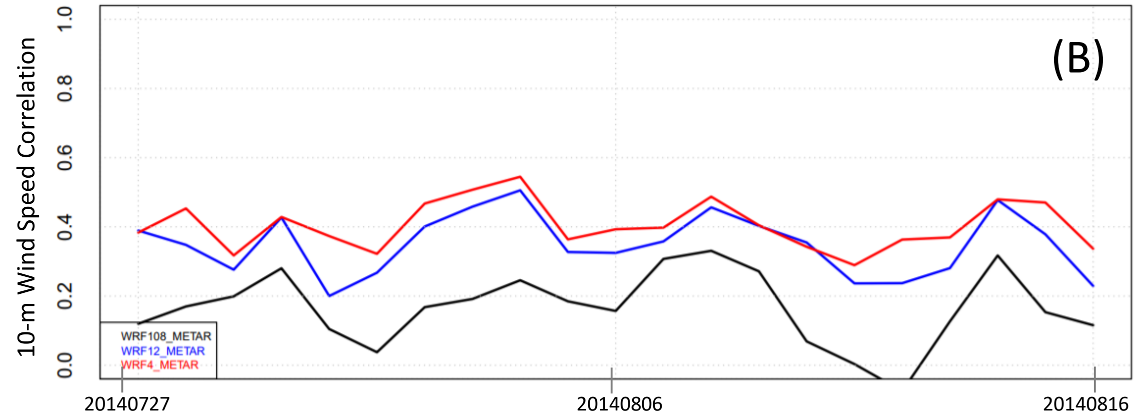


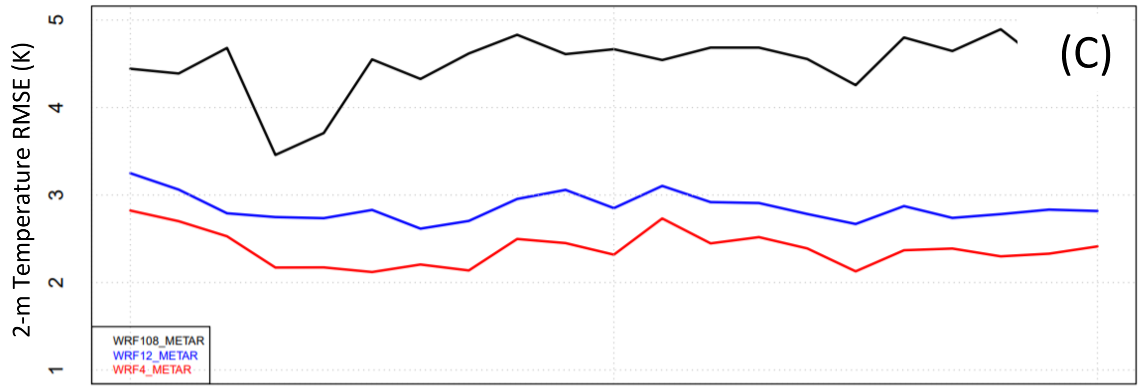
Analyses in presentation focus on:

- Days between July 27, 2014 and August 16, 2014 to align with DISCOVER-AQ/FRAPPE datasets and exclude days potentially impacted by fires; and
- Monitor sites in DMNFR O_3 NAA and a remote site (Figure D).

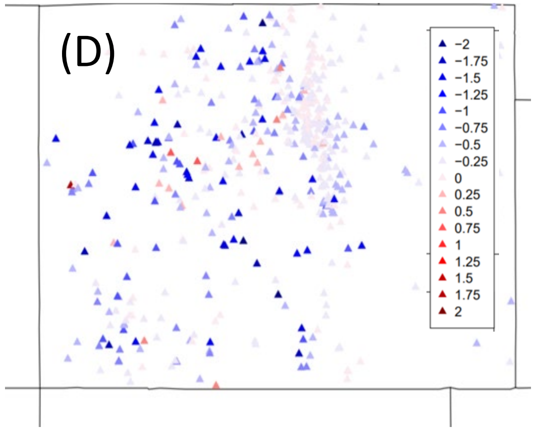
OVERVIEW OF WRF PERFORMANCE:

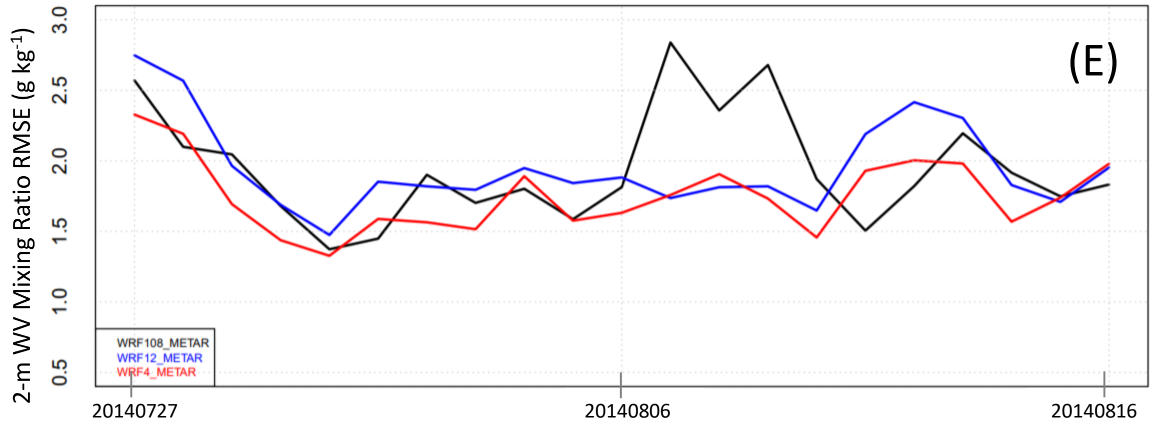






Average Difference in 2-m Temperature RMSE (K) between the 4-km and 12-km Platforms between 07/01/2014 and 08/31/2014.

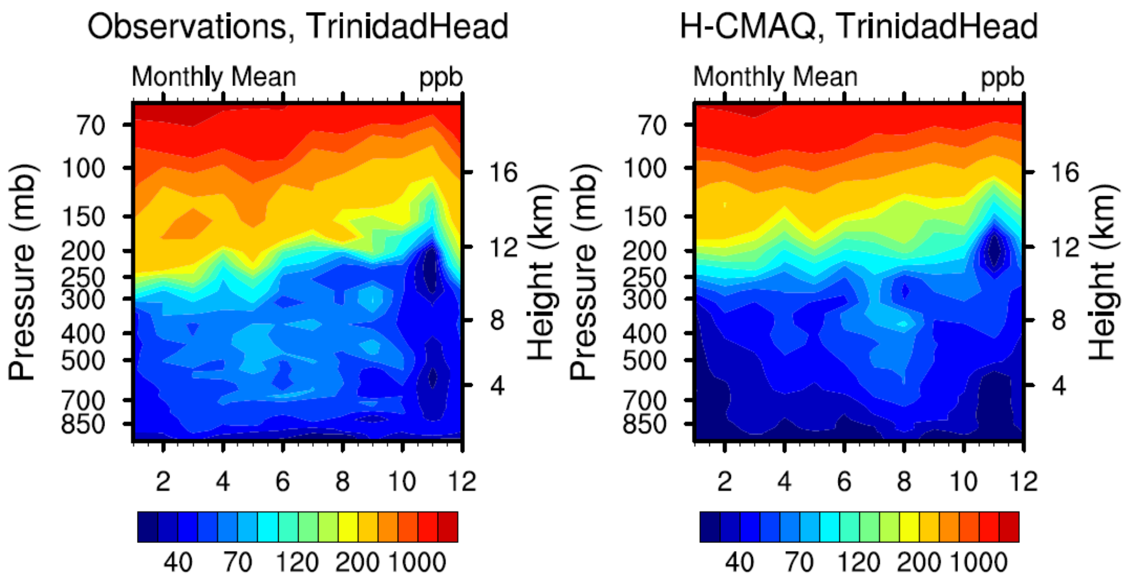




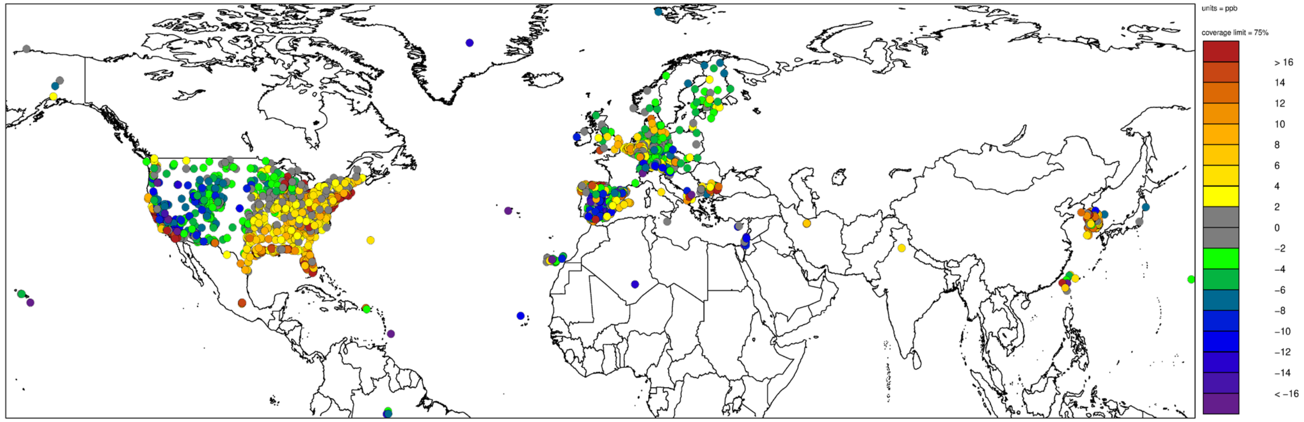
Timeseries of daily average Root Mean Square Error (RMSE) and Correlation (WS only) across METAR sites between 07/27/2014 and 08/16/2014:

- Wind speed is similar among model platforms, but the 4-km platform performs slightly better among the platforms (Figure A & B). The correlation of wind speed (WS) indicates more difference between the platforms, but the the 4-km platform compares the best to the observed signal.
- In areas with complex meteorology (like Colorado), the reduction in grid scale improves the temperature significantly (Figure C & D).
- Mixing ratio has more variable performance among the model platforms, but generally shows that the 4-km platform outperforms the other platforms (Figure E).

OVERVIEW OF H-CMAQ PERFORMANCE FOR O_3:

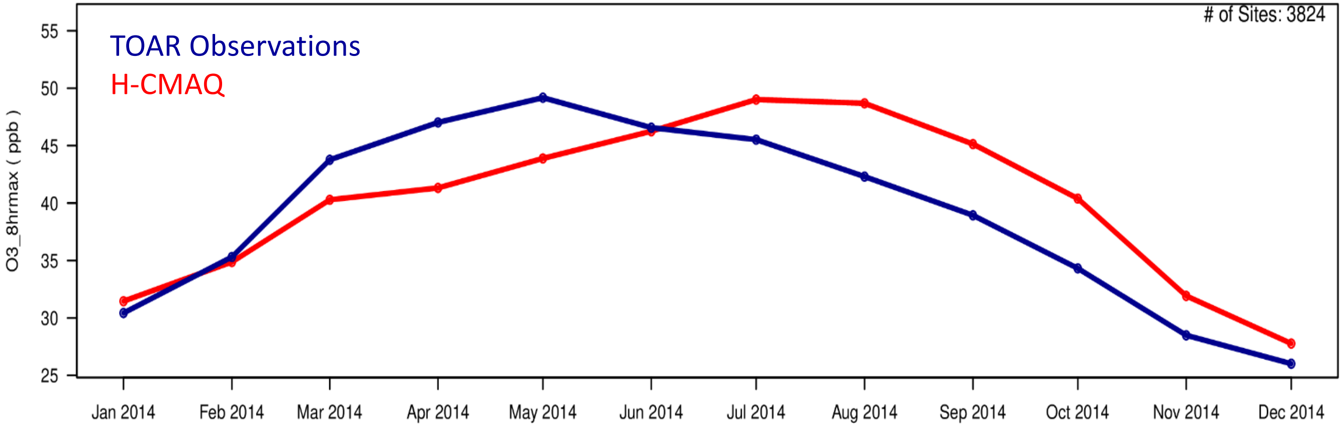


2014 Summer Mean MDA8 O_3, H-CMAQ minus Observations (TOAR)

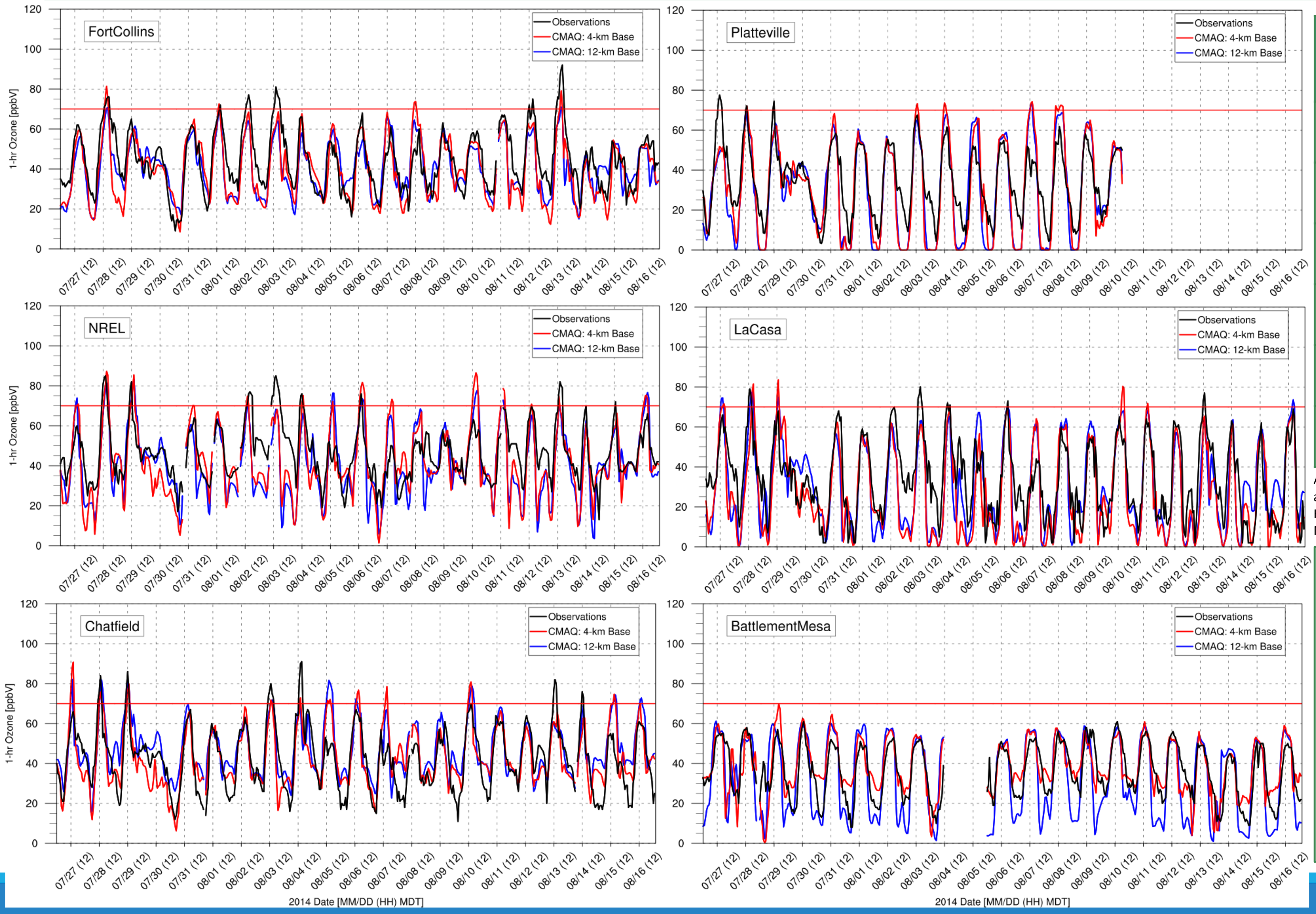


- H-CMAQ performance evaluations used surface observations from:
  - Tropospheric Ozone Assessment Report (TOAR) database, and
  - Ozonesondes from the World Ozone and UV Data Centre (WOUDC) and NOAA archives.
- Examples shown here indicate:
  - Moderate ($\pm$ 5-10 ppb) summertime surface Maximum Daily Average 8-hour (MDA8) O_3 biases,
  - Tendency for H-CMAQ to underestimate surface MDA8 O_3 and free tropospheric O_3 during spring, and
  - Overestimate surface MDA8 O_3 during the second half of the year.

2014 Monthly Mean MDA8 O_3, Observations (TOAR) and H-CMAQ



OVERVIEW OF 12-KM & 4-KM CMAQ PERFORMANCE:



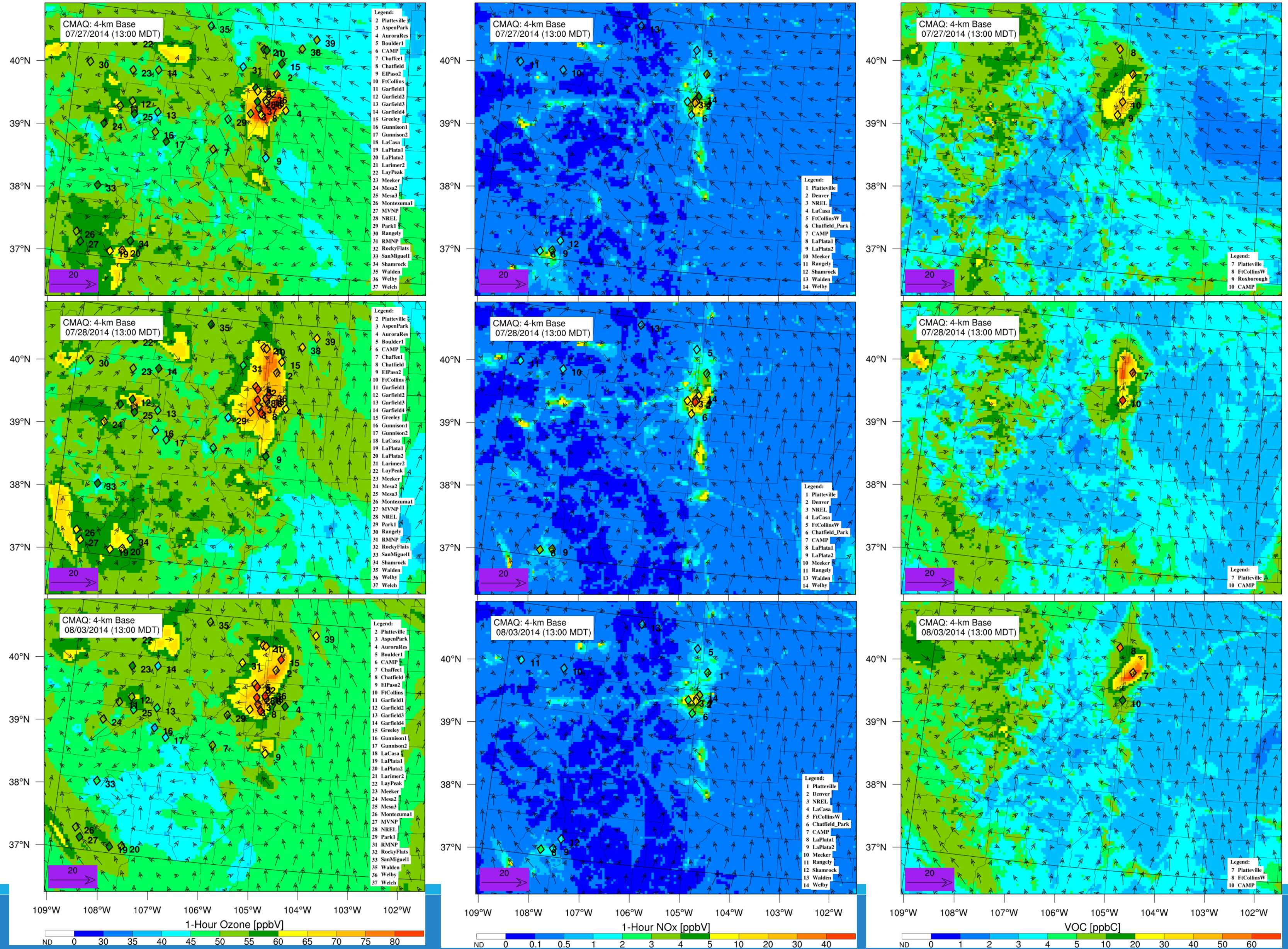
Site	Model Case	O_3 Bias		O_3 RMSE	
		All Days (#)	High O_3 Days (#)	All Days	High O_3 Days
Ft. Collins	4-km	-0.08 (505)	-0.12 (79)	10.25	11.87
	12-km	-0.05 (505)	-0.15 (79)	9.98	12.7
Platteville	4-km	-0.21 (355)	-0.09 (19)	12.47	14.35
	12-km	-0.22 (355)	-0.13 (19)	12.55	14.82
NREL	4-km	-0.09 (500)	-0.06 (80)	13.03	14.21
	12-km	-0.11 (500)	-0.1 (80)	13.13	15.3
LaCasa	4-km	-0.1 (506)	-0.1 (59)	15.19	13.19
	12-km	0.13 (506)	-0.1 (59)	14.36	11.96
Chatfield	4-km	0.07 (503)	-0.06 (75)	10.59	11.58
	12-km	0.18 (503)	-0.04 (75)	11.11	9.82
Battlement Mesa	4-km	0.12 (468)	-0.06 (3)	9.53	5.5
	12-km	-0.14 (468)	-0.04 (3)	13.35	2.63

All Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14. Number of data points in average are noted in parentheses. Units = ppb.
High O_3 Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14 when observed $O_3 \geq 60$ ppb. Number of data points in average are noted in parentheses. Units = ppb.

Timeseries of observed and modeled hourly O_3 between 07/27/2014 and 08/16/2014 at selected sites:

- Model generally captures observed O_3 temporal variability.
- Model is generally biased low for O_3, particularly on days with high O_3 ($\geq$ 60 ppb).
- The 4-km platform generally outperforms the 12-km platform.
- Analyses shown later in presentation will focus on July 27th, July 28th, and August 3rd due to elevated daytime observed O_3 levels and co-located measurements.
- Analyses shown later in presentation will also evaluate O_3 precursors and meteorology to better understand O_3 performance issues.

OVERVIEW OF 4-KM CMAQ PERFORMANCE:



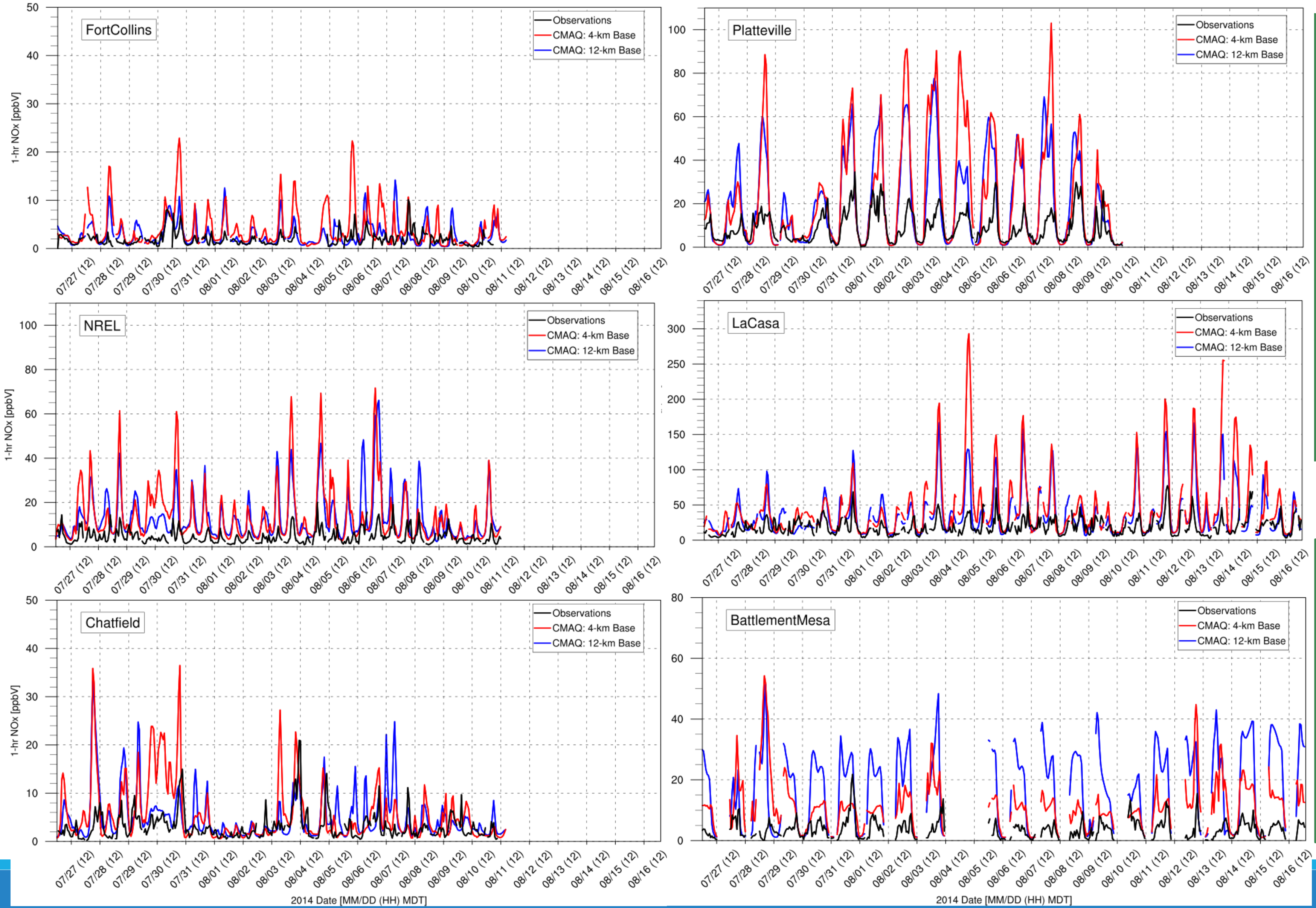
Pollutant/Date	BIAS All Sites (#)	RMSE All Sites
Ozone		
07/27/2014 (13)	0.01 (38)	9.79
07/28/2014 (13)	-0.03 (38)	10.71
08/03/2014 (13)	-0.02 (35)	9.27
NOx		
07/27/2014 (13)	0.19 (14)	4.82
07/28/2014 (13)	0 (13)	13.7
08/03/2014 (13)	0.3 (14)	3.14
VOC		
07/27/2014 (13)	-0.4 (4)	22.86
07/28/2014 (13)	-0.59 (2)	36.88
08/03/2014 (13)	-0.38 (3)	29.08

BIAS and RMSE: Average among sites with observations in Colorado. Values in parentheses represent the number of data points in averages. Units = ppb.

Observed and modeled O_3 (1st Column), NOx (2nd Column), and VOC (3rd Column) on July 27th (1st row), July 28th (2nd row), and August 3rd (3rd row) at 1pm local across Colorado (wind vectors simulated by model also shown):

- Model appears to generally capture the spatial extent of the elevated O_3, NOx, and VOC, except for the observed elevated O_3 levels in the northeast portion of the DMNFR NAA.
- Model is generally biased low for O_3 and VOC and biased high for NOx.
- Issues with the emissions and meteorology could be contributing to model performance issues, and further investigated later in presentation.

OVERVIEW OF 12-KM & 4-KM CMAQ PERFORMANCE:



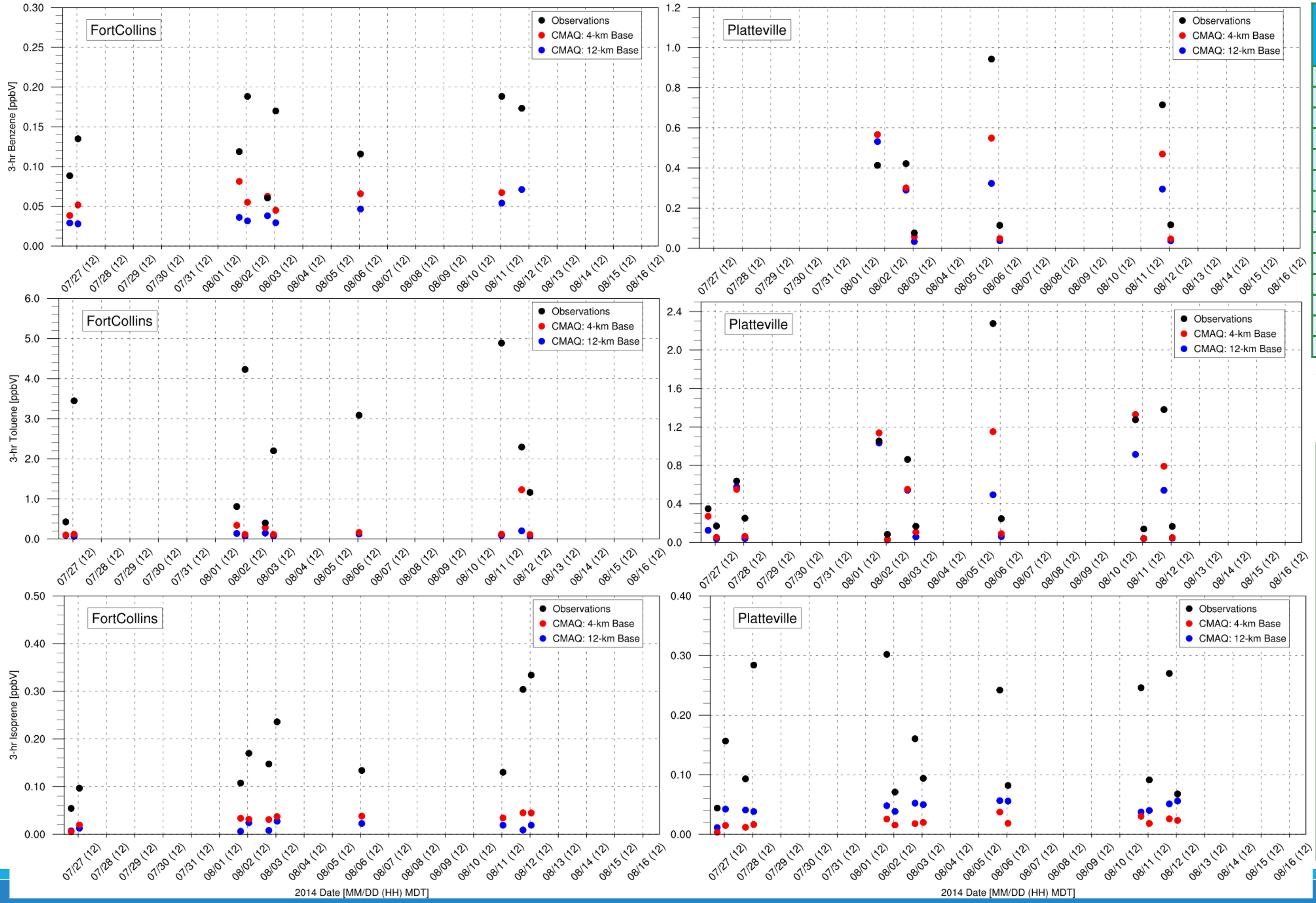
Site	Model Case	NOx Bias		NOx RMSE	
		All Days (#)	High O_3 Days (#)	All Days	High O_3 Days
Ft. Collins	4-km	3.74 (319)	1.68 (53)	4.27	3.53
	12-km	3.25 (319)	0.69 (53)	2.56	1.98
Platteville	4-km	1.37 (352)	-0.34 (19)	24.67	2.38
	12-km	1.21 (352)	-0.51 (19)	20.11	2.24
NREL	4-km	2.67 (359)	1.84 (55)	15.1	7.77
	12-km	2.52 (359)	2.15 (55)	13.18	8.67
LaCasa	4-km	1.5 (478)	0.68 (59)	46.28	10.69
	12-km	1.01 (478)	0.42 (59)	30.6	7.2
Chatfield	4-km	1.4 (354)	0.75 (53)	6.3	3.71
	12-km	1.28 (354)	0.99 (53)	5.23	3.62
Battlement Mesa	4-km	7.96 (381)	3.41 (1)	11.11	1.36
	12-km	9.24 (381)	2.33 (1)	18.29	0.93

All Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14. Number of data points in average are noted in parentheses. Units = ppb.
High O_3 Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14 when observed $O_3 \geq 60$ ppb. Number of data points in average are noted in parentheses. Units = ppb.

Timeseries of observed and modeled hourly NOx between 07/27/2014 and 08/16/2014 at selected sites:

- Model generally captures the temporal variability observed by measurements, but the model is biased high.
- The 12-km model platform performs slightly better relative to the 4-km model platform. This could be a result of the model resolution, where the NOx emissions are being spread across a larger area in the 12-km platform, thereby reducing the overall NOx emissions.
- **Results suggest that the emissions inventory could be contributing to the O_3 performance issues.**

OVERVIEW OF 12-KM & 4-KM CMAQ PERFORMANCE:



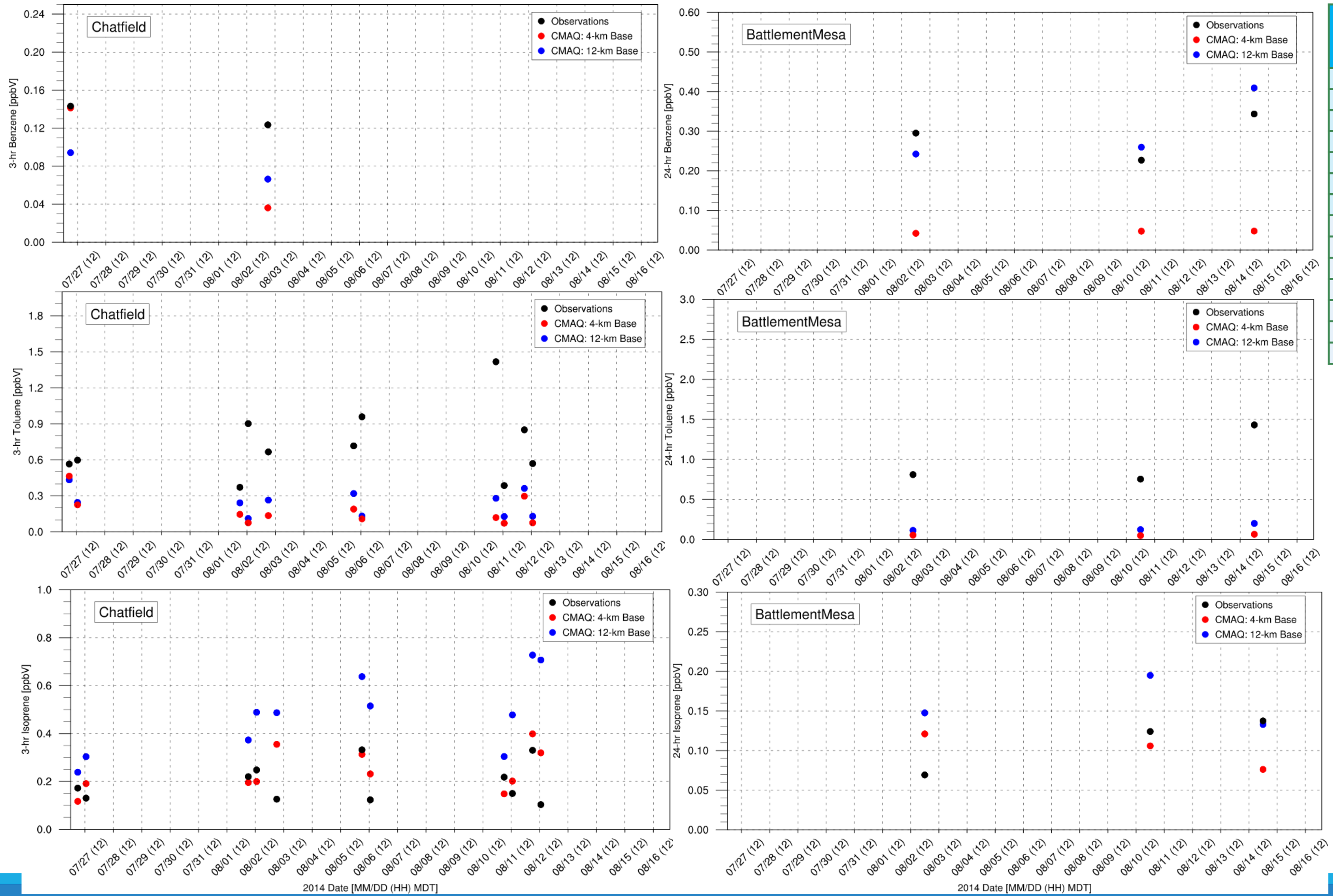
Site/Pollutant	VOC BIAS			
	4-km Base		12-km Base	
	All Days (#)	High O_3 Days (#)	All Days	High O_3 Days
Ft. Collins				
Benzene	-0.31 (9)	-0.62 (4)	-0.67	-0.74
Toluene	-0.78 (10)	-0.95 (5)	-0.89	-0.96
Ethane	-0.29 (10)	-0.23 (5)	-0.44	-0.29
Xylene	-0.01 (10)	-0.27 (5)	-0.56	-0.51
Formaldehyde	NA	NA	NA	NA
Isoprene	-0.79 (10)	-0.79 (5)	-0.89	-0.87
Platteville				
Benzene	-0.3 (7)	-0.24 (1)	-0.45	-0.56
Toluene	-0.43 (14)	-0.6 (3)	-0.57	-0.76
Ethane	0.94 (14)	0.26 (3)	0.89	0.09
Xylene	-0.64 (14)	-0.87 (3)	-0.71	-0.91
Formaldehyde	-0.08 (14)	-0.48 (3)	-0.26	-0.57
Isoprene	-0.84 (14)	-0.87 (3)	-0.63	-0.68

All Days (#): Average Bias between 07/27/14 and 08/16/14. Number of data points in average are noted in parentheses. Units = ppb.

High O_3 Days (#): Average Bias between 07/27/14 and 08/16/14 when observed $O_3 \geq 60$ ppb. Number of data points in average are noted in parentheses. Units = ppb.

- Timeseries of observed and modeled 3-hour speciated VOCs between 07/27/2014 and 08/16/2014 at Fort Collins and Platteville. The 3-hour measurements were started at 6am and 1pm local.
- Table presents statistical information for additional speciated VOCs. VOCs analyses for additional sites are presented on next slide.
- Sites and speciated VOCs were selected based on available datasets and VOCs that are highly reactive.
- **Analyses presented here suggest:**
  - **Models are generally biased low, except for ethane at Platteville.**
  - **4-km platform performs better than the 12-km platform.**

OVERVIEW OF 12-KM & 4-KM CMAQ PERFORMANCE:



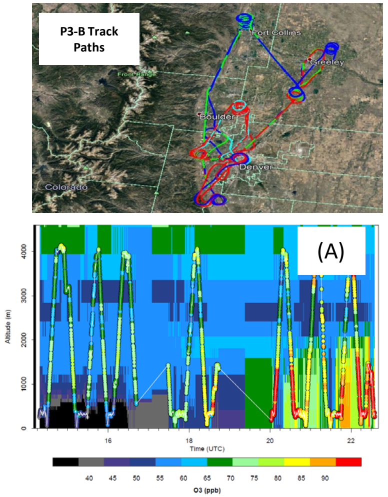
Site/Pollutant	VOC BIAS			
	4-km Base		12-km Base	
	All Days (#)	High O_3 Days (#)	All Days	High O_3 Days
Chatfield				
Benzene	-0.36 (2)	0 (0)	-0.4	0
Toluene	-0.72 (11)	-0.79 (4)	-0.62	-0.72
Ethane	0.01 (11)	0.35 (4)	-0.22	-0.09
Xylene	-0.73 (11)	-0.85 (4)	-0.58	-0.72
Formaldehyde	0.54 (12)	1.74 (5)	0.59	1.95
Isoprene	0.43 (11)	0.94 (4)	1.81	3.13
Battlement Mesa				
Benzene	-0.83 (3)	0 (0)	0.05	0
Toluene	-0.94 (3)	0 (0)	-0.85	0
Ethane	-0.67 (3)	0 (0)	-0.46	0
Xylene	-0.93 (3)	0 (0)	-0.8	0
Formaldehyde	0.1 (2)	0 (0)	0	0
Isoprene	0.05 (3)	0 (0)	0.55	0

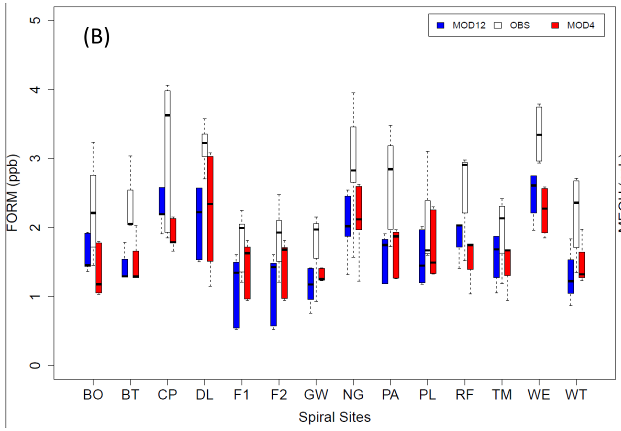
All Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14. Number of data points in average are noted in parentheses. Units = ppb.
High O_3 Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14 when observed $O_3 \geq 60$ ppb. Number of data points in average are noted in parentheses. Units = ppb.

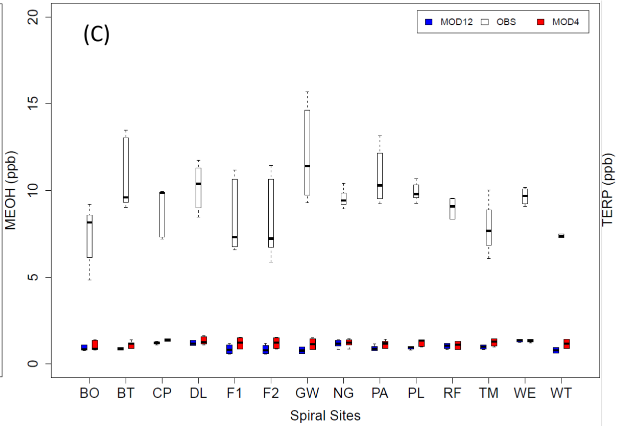
- Timeseries of observed and modeled 3-hour/24-hour speciated VOCs between 07/27/2014 and 08/16/2014 at Chatfield and Battlement Mesa. The 3-hour measurements were started at 6am and 1pm local, while the 24-hour measurements started at midnight.
- Table presents statistical information for additional speciated VOCs.
- Overall, analyses suggest:
  - Models are generally bias low for speciated VOCs, except for ethane at Platteville and Chatfield and formaldehyde and isoprene at Battlement Mesa.
  - 4-km platform performs better than the 12-km platform.
  - **Results suggest that the emissions inventory could be contributing to the O_3 performance issues and grid resolution better resolves the predicted impacts.**

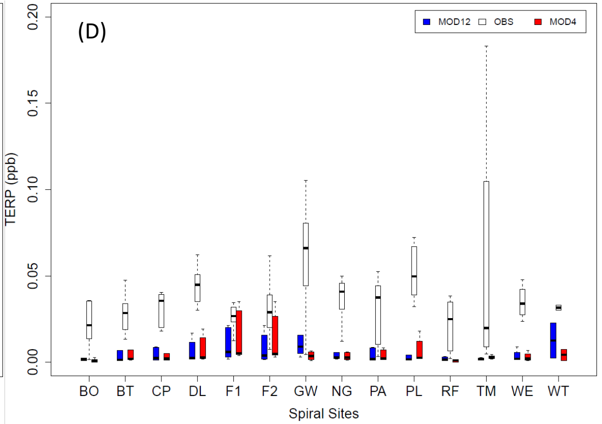
OVERVIEW OF 12-KM & 4-KM CMAQ PERFORMANCE:

July 28, 2014: P3-B Aircraft Data Comparisons to 4-km and 12-km Model Platforms for (A) Ozone, (B) Formaldehyde, (C) Methanol, (D) Terpene







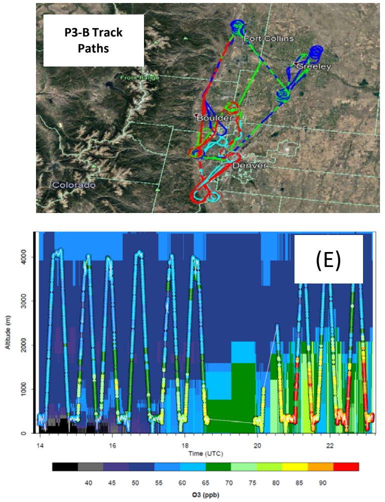


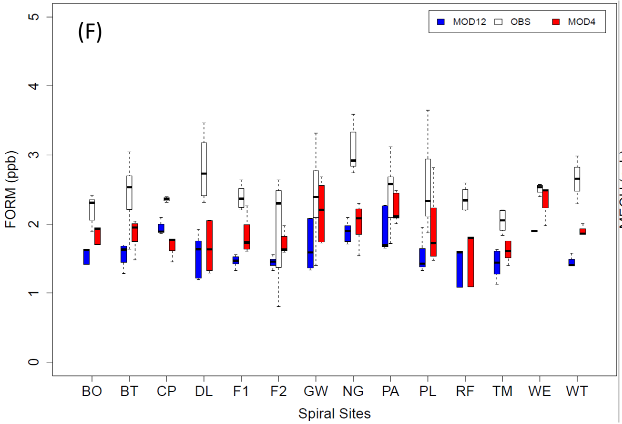
(A): Curtain plot shows O_3 from aircraft along track paths and the relative modeled O_3. (B) through (D): Box plots show average values over entire spirals at various locations. Results align with (A), where maximum height is about 4 km above ground level (AGL).
Legend: BO = Boulder; BT = BAO Tower; CP = Chatfield Park; DL = Denver-LaCasa; F1 = Ft. CollinsW; F2 = Ft. CollinsW2; GW = Greeley-Weld; NG = NREL-Golden; PA = Parkland Airstrip; PL=Platteville; RF=RockyFlats; TM=TableMtn; WE = Welch; WT = WeldTower

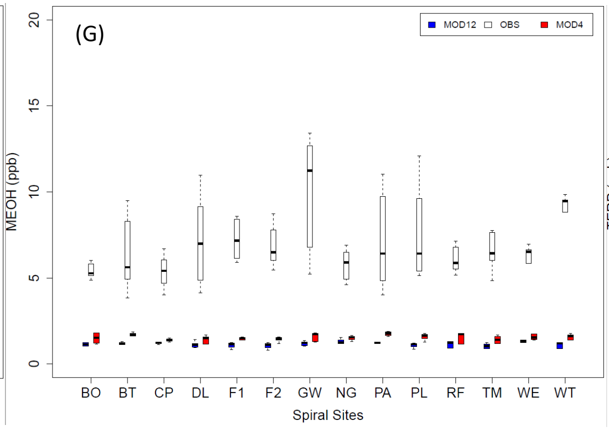
Model biased low for O_3 and selected VOCs.

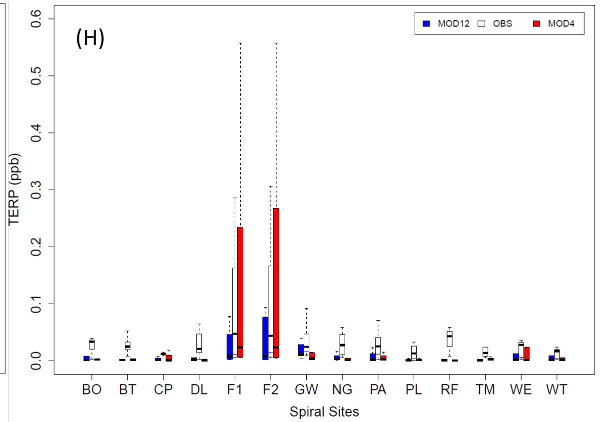
Model did not capture vertical distribution of O_3 observed by P3-B.

August 3, 2014: P3-B Aircraft Data Comparisons to 4-km and 12-km Model Platforms for (E) Ozone, (F) Formaldehyde, (G) Methanol, (H) Terpene





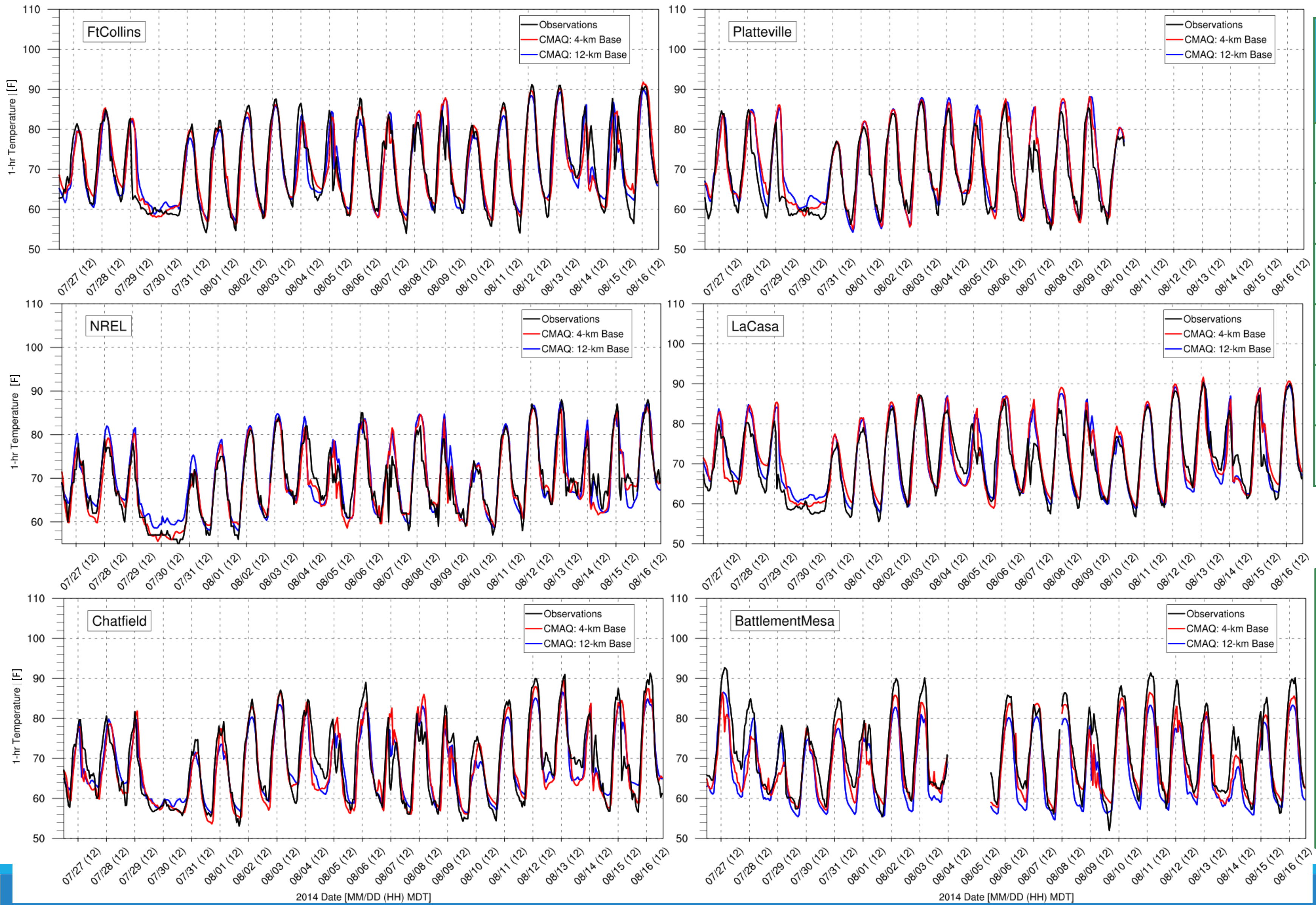




(E): Curtain plot shows O_3 from aircraft along track paths and the relative modeled O_3. (F) through (H): Box plots show average values over entire spirals at various locations. Results align with (E), where maximum height is about 4 km AGL.
Legend: BO = Boulder; BT = BAO Tower; CP = Chatfield Park; DL = Denver-LaCasa; F1 = Ft. CollinsW; F2 = Ft. CollinsW2; GW = Greeley-Weld; NG = NREL-Golden; PA = Parkland Airstrip; PL=Platteville; RF=RockyFlats; TM=TableMtn; WE = Welch; WT = WeldTower

Improvements to emissions inventory and meteorological model could address model performance issues.

OVERVIEW OF 12-KM & 4-KM WRF PERFORMANCE:



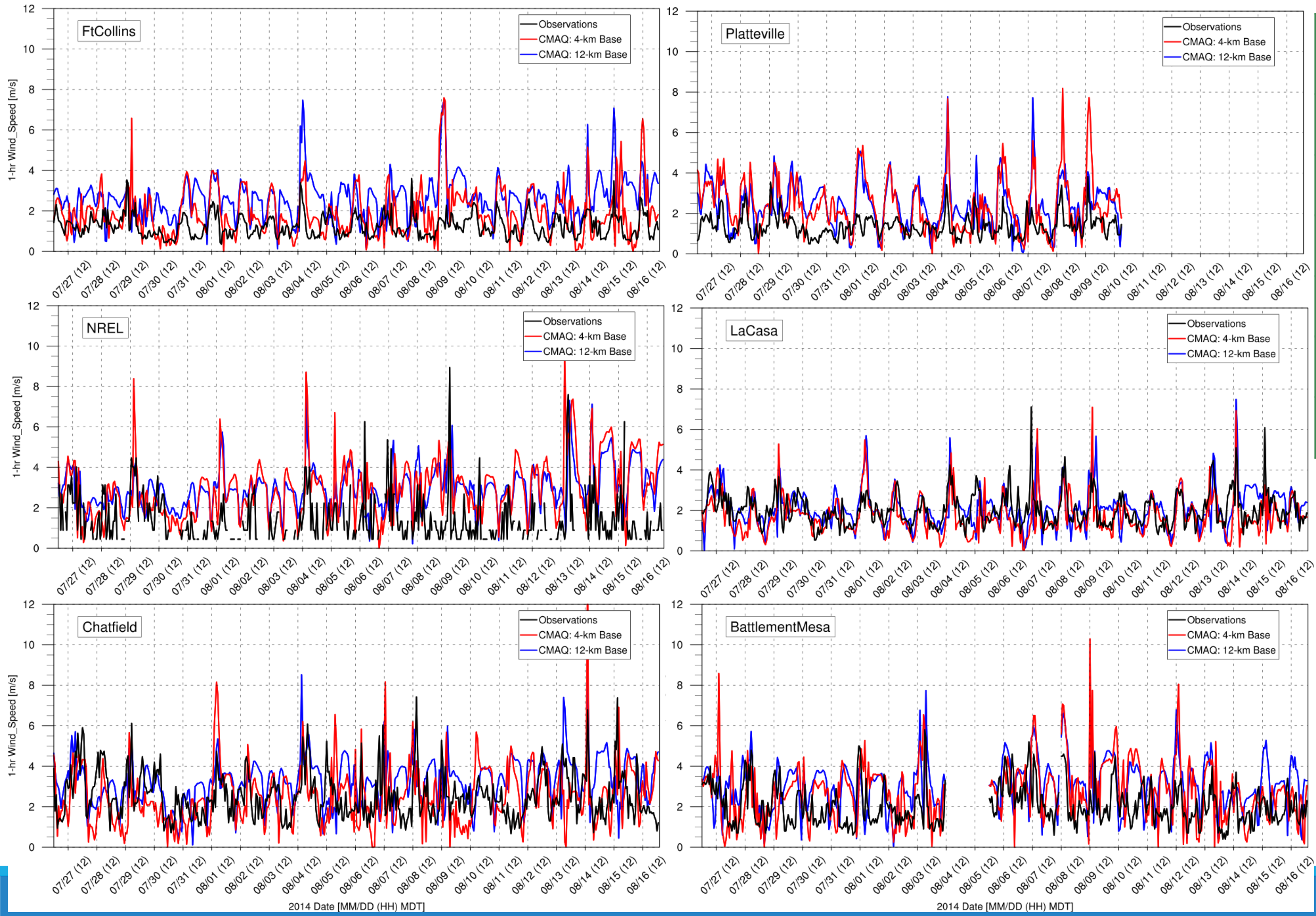
Site	Model Case	Temperature Bias		Temperature RMSE	
		All Days (#)	High O_3 Days (#)	All Days	High O_3 Days
Ft. Collins	4-km	0.001 (506)	-0.01 (47)	4.22	2.61
	12-km	-0.003 (506)	-0.02 (47)	3.63	2.41
Platteville	4-km	0.01 (355)	-0.01 (19)	4.58	2.8
	12-km	0.02 (355)	-0.01 (19)	4.45	2.76
NREL	4-km	-0.002 (498)	-0.01 (79)	2.98	3.14
	12-km	0.01 (498)	0.01 (79)	3.28	3.02
LaCasa	4-km	0.01 (506)	0.01 (59)	4.09	2.58
	12-km	0.009 (506)	0.01 (59)	3.59	2.18
Chatfield	4-km	-0.01 (506)	-0.02 (75)	4.33	3.58
	12-km	-0.008 (506)	-0.04 (75)	3.92	4.37
Battlement Mesa	4-km	-0.03 (469)	-0.03 (3)	4.34	3
	12-km	-0.05 (469)	-0.05 (3)	5.23	5.12

All Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14. Number of data points in average are noted in parentheses. Units = Fahrenheit.
High O_3 Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14 when observed $O_3 \geq 60$ ppb. Number of data points in average are noted in parentheses. Units = Fahrenheit.

Timeseries of observed and modeled hourly **temperature** between 07/27/2014 and 08/16/2014 at selected sites:

- Model captures the temporal variability of the observed temperatures.
- At these sites, the performance among the platforms are mixed, but overall the 4-km platform performs slightly better than the 12-km platform, especially in mountain areas.
- The modeled temperatures are slightly cooler relative to the observations, but the magnitude of the bias is not anticipated to significantly impact the ozone formation.

OVERVIEW OF 12-KM & 4-KM WRF PERFORMANCE:



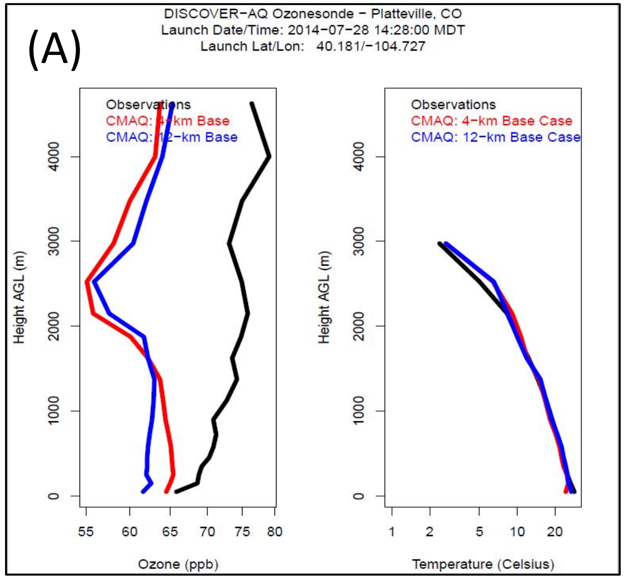
Site	Model Case	Wind Speed Bias		Wind Speed RMSE	
		All Days (#)	High O_3 Days (#)	All Days	High O_3 Days
Ft. Collins	4-km	0.64 (506)	0.75 (47)	1.24	1.37
	12-km	1.48 (506)	0.78 (47)	1.73	1.28
Platteville	4-km	0.87 (355)	0.96 (19)	1.57	1.53
	12-km	0.89 (355)	0.86 (19)	1.45	1.36
NREL	4-km	2.32 (416)	1.74 (76)	2.33	2.1
	12-km	2.34 (416)	1.78 (76)	2.15	1.73
LaCasa	4-km	-0.09 (506)	-0.11 (59)	0.97	0.98
	12-km	0.14 (506)	-0.03 (59)	0.92	0.82
Chatfield	4-km	0.17 (506)	-0.1 (75)	1.6	1.49
	12-km	0.53 (506)	0.27 (75)	1.62	1.35
Battlement Mesa	4-km	0.57 (469)	0.56 (3)	1.62	1.58
	12-km	0.76 (469)	0.15 (3)	1.64	1.43

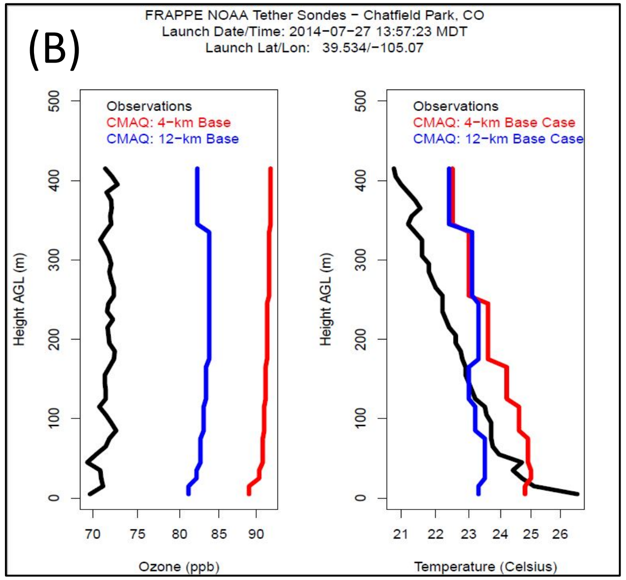
All Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14. Number of data points in average are noted in parentheses. Units = Meters Per Second.
High O_3 Days (#): Average Bias and RMSE between 07/27/14 and 08/16/14 when observed $O_3 \geq 60$ pp. Number of data points in average are noted in parentheses. Units = Meters Per Second.

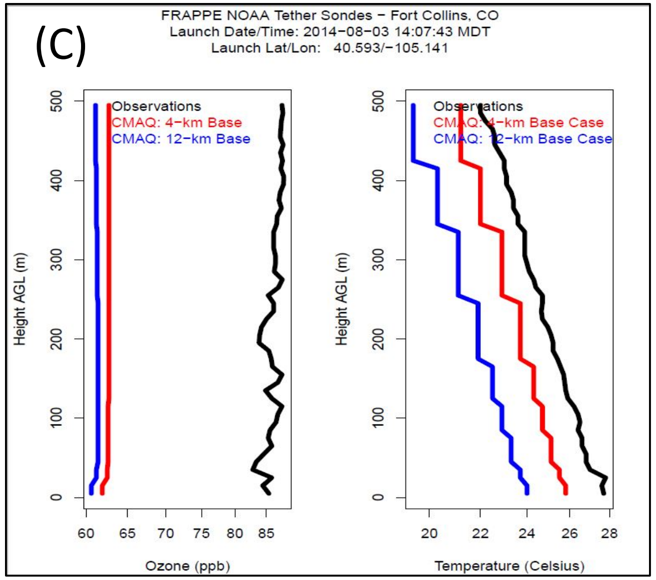
Timeseries of observed and modeled hourly **wind speed** between 07/27/2014 and 08/16/2014 at selected sites:

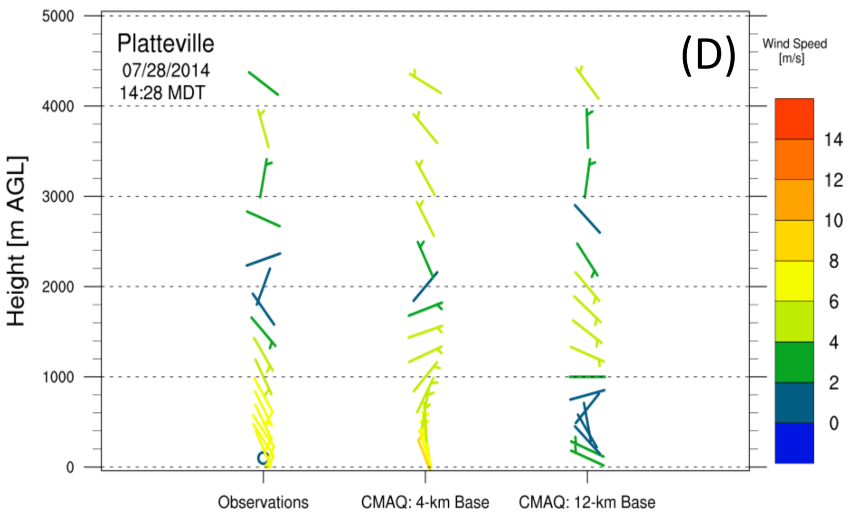
- Modeled wind speed does not consistently track the observed temporal variability.
- The models are generally biased high or have higher wind speeds relative to the observations.
- The 4-km platform generally performs better than the 12-km platform, especially considering the correlation shown in slide 4.
- **Analyses suggest issues with the meteorological model, where the higher modeled wind speeds could indicate a deeper planetary boundary layer (PBL) and/or stronger ventilation of pollutants in PBL. These issues could contribute to the under-predictions of O_3 and its precursors shown in previous slides.**

OVERVIEW OF 12-KM & 4-KM CMAQ PERFORMANCE:









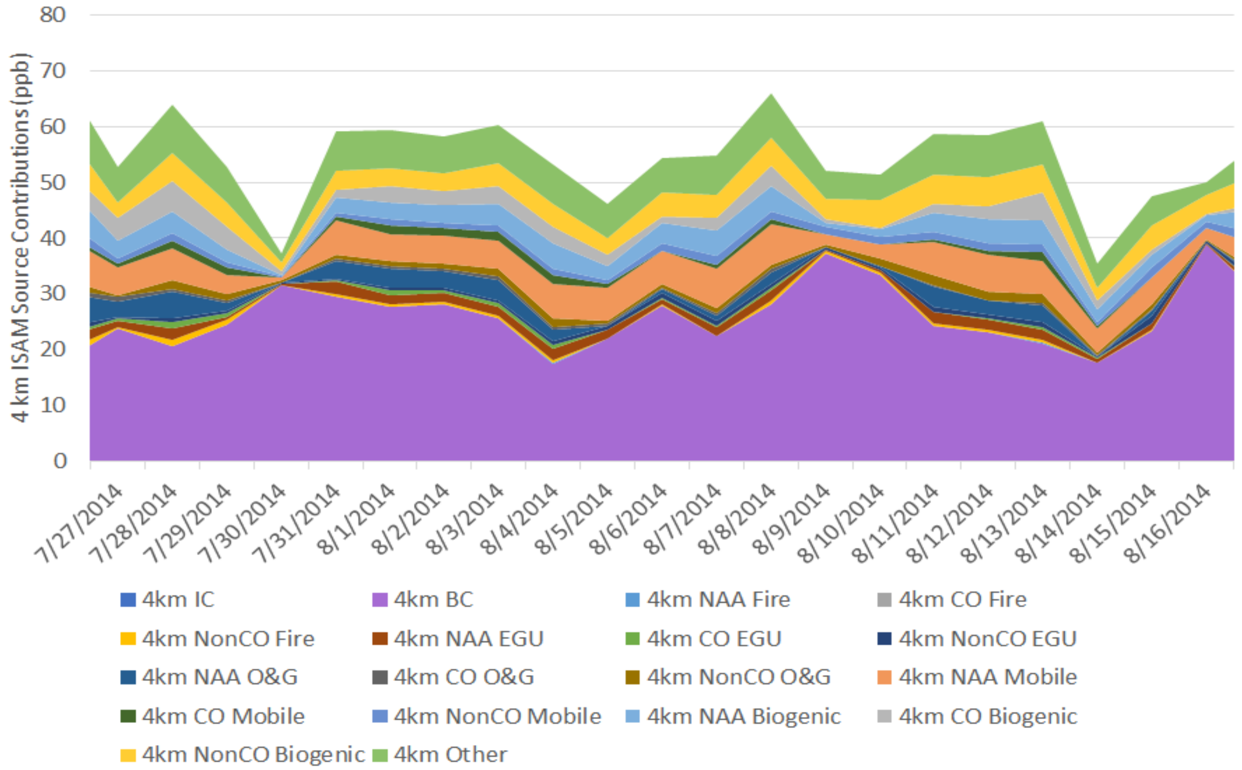
Vertical profiles of observed and modeled O_3 and Temperature at (A) Platteville, (B) Chatfield, and (C) Fort Collins on July 28th, July 27th, and August 3rd, respectively, around 2pm local (vertical profiles of WS & WD at Platteville (D) also shown):

- **Platteville (A&D):** While vertical structure of temperature predicted by models compare well to observations at Platteville, the vertical structure of O_3 does not (A). At this site, the magnitude of the 4-km modeled O_3 at the surface is similar to the observations, but the low bias increases with increasing altitude (A). Comparisons of wind speed and direction (D) also show that the modeled 4-km wind speed profile is similar to the observations, but the wind direction is different. **These results suggest that the meteorological model could be impacting the low-level transport (i.e., more than vertical mixing) of the 4-km O_3 and its precursors.**
- **Chatfield (B):** Vertical structure of modeled O_3 at Chatfield is similar to the observations, but the model is biased high. Temperature profiles at this site indicate that the models have stronger mixing relative to the observations. Timeseries shown in slide 13 also indicates that the modeled wind speed is biased low at the surface at this site. **These results suggest that the modeled vertical mixing and low-level transport could be impacting the modeled O_3 precursors (i.e., contributing to higher modeled O_3 relative to the observations).**
- **Ft. Collins (C):** Vertical structure of modeled O_3 at Ft. Collins is similar to the observations, but the model is biased low. Temperature profiles indicate a difference in temperatures between the models and observations, but the structures of the profiles are similar. Timeseries shown in slide 13 also indicate that the modeled wind speed is biased high at the surface at this site. **This suggests that the mixing in the model should be similar to the observations, but the low-level transport could be impacting O_3 and its precursors.**

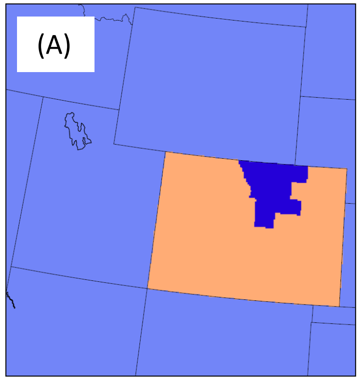
OVERVIEW OF CMAQ-ISAM RESULTS:

The model platforms utilized CMAQ v5.3.2 that included ISAM (CMAQ-ISAM) to track emission contributions from various source sectors and portions of the model domains (i.e., source regions). The geographic scope of defined source regions and granularity of tracked emission sources was finest for the 4-km CMAQ-ISAM simulation and became successively more aggregated for the 12-km and 108-km simulations (A-C). The 4-km CMAQ-ISAM simulation was configured to track source contributions to O_3 formation from 5 sectors (mobile, EGU, oil & gas, biogenics, and fires) and 3 regions (DMNFR NAA, Colorado [excluding DMNFR NAA], and Non-Colorado).

Example: ISAM Contributions at Time of MDA8 O_3
Fort Collins between July 27, 2014 and August 16, 2014

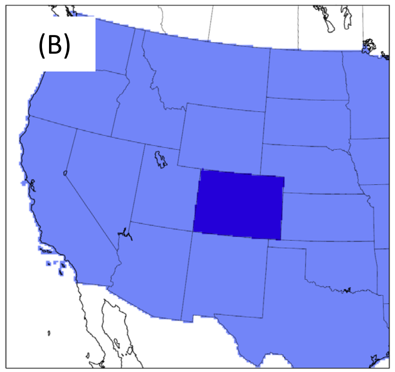


CMAQ 4km ISAM Regions



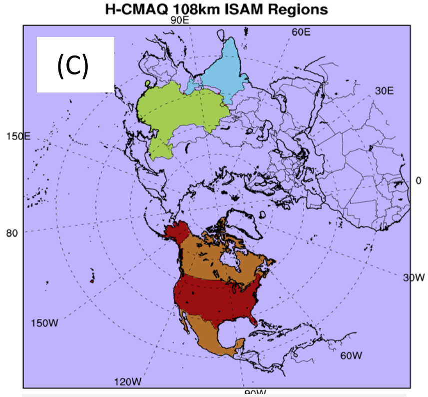
18 Tags: 3 source regions, 5 emission sectors, plus IC, BC, other

CMAQ 12km ISAM Regions



13 Tags: 2 source regions (Non-Colorado, Colorado), 5 emission sectors (biogenics, fires, EGUs, mobile, O&G), plus IC, BC, other

H-CMAQ 108km ISAM Regions



16 Tags: 5 source regions (US, Non-US, China, Mexico/Canada), 5 emission sectors (Biogenics, Fires, Shipping, O3-PV, Anthropogenic), plus stratosphere, IC, BC, other)

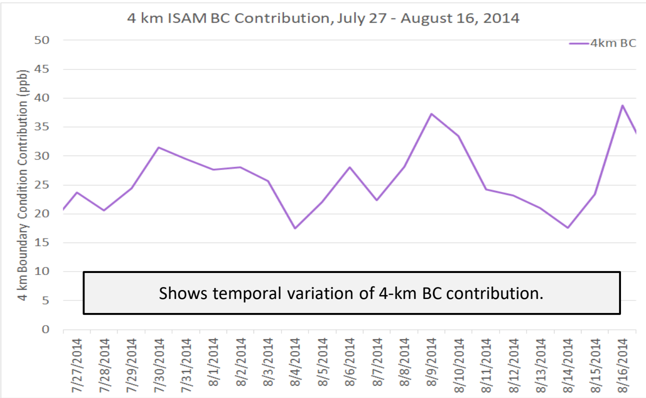
The 4-km CMAQ-ISAM Model Simulation Results:

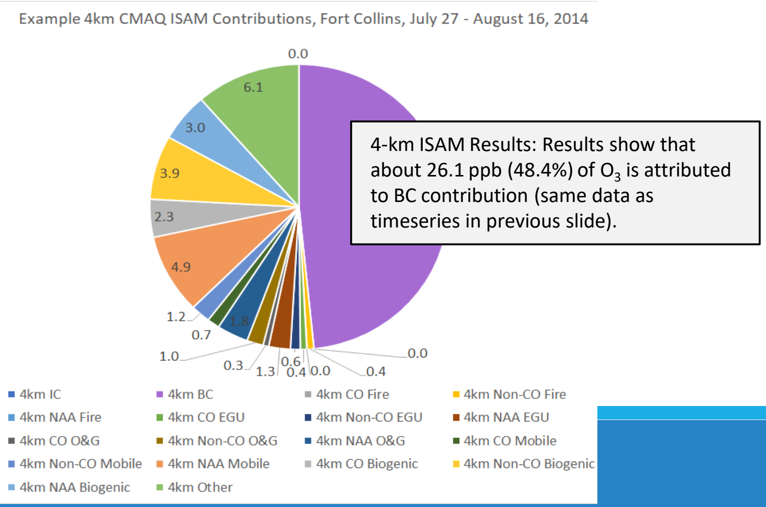
- Illustrate day-to-day variability in sector and region contributions.
- Average Top 6 Contributors: Boundary Conditions (BC), other sectors, non-Colorado biogenic, Colorado biogenic, Colorado Mobile, DMNFR NAA Mobile.
- Large contribution from BC. To characterize BC contributions for the 4-km platform: (1) Used inert boundary tracers on the 4-km and 12-km platforms and (2) Ran ISAM for the 12-km and 108-km platforms. Analysis shown on next slide.

OVERVIEW OF CMAQ-ISAM RESULTS:

ISAM does not currently support nesting of source attribution results across multiple grids. A method was developed to use the ISAM results from the coarser grids (i.e., 12-km and 108-km platforms) and implement inert BC tracers on the finer grids (12-km and 4-km platforms) to estimate which coarser-grid sectors and regions contribute to the finer-grid BC contribution (i.e., better understand break-down of the 4-km CMAQ-ISAM BC contribution).

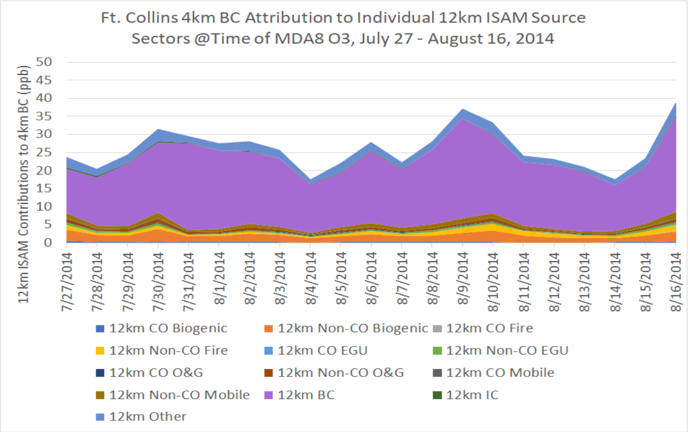
4-km CMAQ-ISAM Model Platform

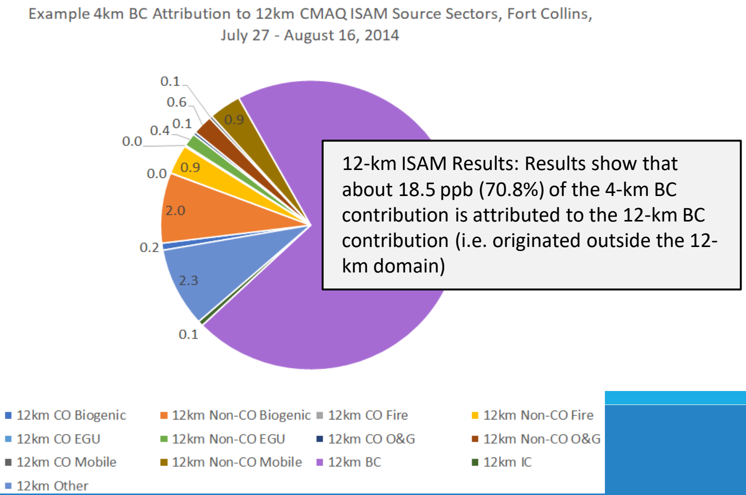




4-km ISAM Results: Results show that about 26.1 ppb (48.4%) of O_3 is attributed to BC contribution (same data as timeseries in previous slide).

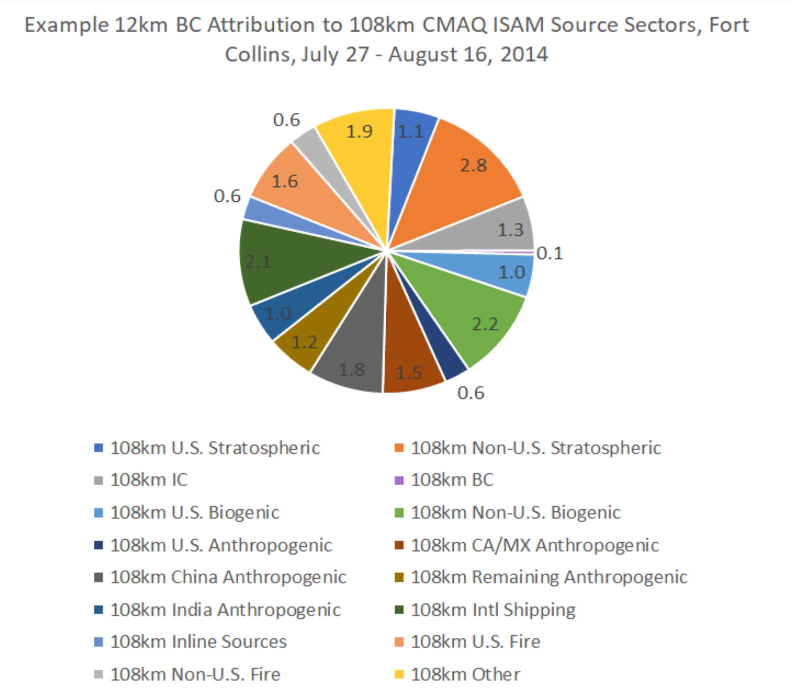
12-km CMAQ-ISAM Model Platform





12-km ISAM Results: Results show that about 18.5 ppb (70.8%) of the 4-km BC contribution is attributed to the 12-km BC contribution (i.e. originated outside the 12-km domain)

108-km CMAQ-ISAM Model Platform



108-km ISAM Results: Results show that a variety of anthropogenic and natural sources contribute to the 12-km ISAM BC estimate, including stratospheric O_3. The largest contributions were from the stratosphere, biogenic sources outside the U.S., and international shipping.

CONCLUSIONS & FUTURE WORK:

- DISCOVER-AQ and FRAPPE datasets provide a unique opportunity to conduct comprehensive diagnostic model evaluations, including:
  - Co-located measurements with multiple air pollutant and meteorological variables captured at multiple spatial, temporal, and vertical scales; and
  - Speciated VOCs and NOx measurements.
- Overview of Model Performance
  - Model generally captures the temporal variability and spatial extent of the observed pollutants and meteorological parameters, but the model has difficulty capturing the vertical distribution and structure of O_3 and some meteorological parameters.
  - Model is generally biased low for O_3 and many speciated VOCs, while biased high for NOx, between July 27 and August 16, 2014 and on days with high O_3 levels (i.e., $\geq$ 60 ppb). The model bias is variable at some sites for Ethane, Formaldehyde, and Isoprene.
  - Relative to observations, the model is slightly cooler, with higher wind speeds.
  - Model performance improves with finer resolution (i.e., 4-km model platform relative to 12-km model platform).
  - Evaluation suggests that the O_3 performance issues could be a result of issues with the emissions inventory and precursor transport driven by the meteorological model.
- Ozone Source Apportionment
  - Results from the 4-km CMAQ-ISAM simulation illustrate day-to-day variability in sector and region contributions to O_3 formation, and a large contribution from boundary conditions. However, the negative bias for O_3 indicates that the model might underestimate local contributions to O_3. More work needs to be completed to understand the ISAM contributions to O_3 given the uncertainty in the model performance.
  - Developed approach that nested source attribution results across multiple grids to better understand which coarser-grid source sectors and regions attribute to the finer-grid boundary conditions contribution to O_3.
- Future Work
  - Sensitivity studies to further investigate emissions, including refined emissions for Oil & Gas and Volatile Chemical Products (VCPs).
  - Sensitivity studies to further investigate meteorology, including vertical coordinate configuration options and land-surface and PBL representation.

ACKNOWLEDGEMENTS:

- DISCOVER-AQ and FRAPPE Teams for the Extensive Dataset Collection:
  - P-3B Aircraft Datasets: Andy Weinheimer (UCAR), Jim Crawford (NASA), Gao Chen (NASA), and Michael Shook (NASA)
  - NASA/PSU Ozonesondes Datasets (Platteville): Anne Thompson (NASA) and Bill Brune (PSU)
  - NOAA Balloon Tether Ozone Datasets (Denver, Chatfield, Ft. Collins): Bryan Johnson and Patrick Cullis
  - EPA Surface NOx Datasets (Chatfield, Ft. Collins, and NREL): Russell Long
  - CDPHE Surface NOx Datasets (Denver and LaCasa): Erick Mattson (CDPHE – Air Pollution Control Division)
  - Speciated Surface VOC Datasets: Collected by CDPHE and available in EPA's AQS.
- EPA Air Quality System (AQS) Database: https://www.epa.gov/aqs
- METAR Datasets: https://madis.ncep.noaa.gov/madis_sfc.shtml
- TOAR Surface Ozone Observations: Schultz MG, Schröder S, Lyapina O, Cooper O, Galbally I, et al. 2017. Tropospheric Ozone Assessment Report: Database and metrics data of global surface ozone observations. Elementa. DOI:10.1525/elementa.244
- Ozonesonde Dataset for H-CMAQ: World Ozone and UV Data Centre (http://www.woudc.org), NOAA Earth Systems Research Laboratories (ftp://aftp.cmdl.noaa.gov/data/ozwv/Ozonesonde; https://www.esrl.noaa.gov/gmd/ozwv/ozsondes/index.html)

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