Evaluation of the Community Multiscale Air Quality Model for Simulating Winter Ozone Formation in the Uinta Basin

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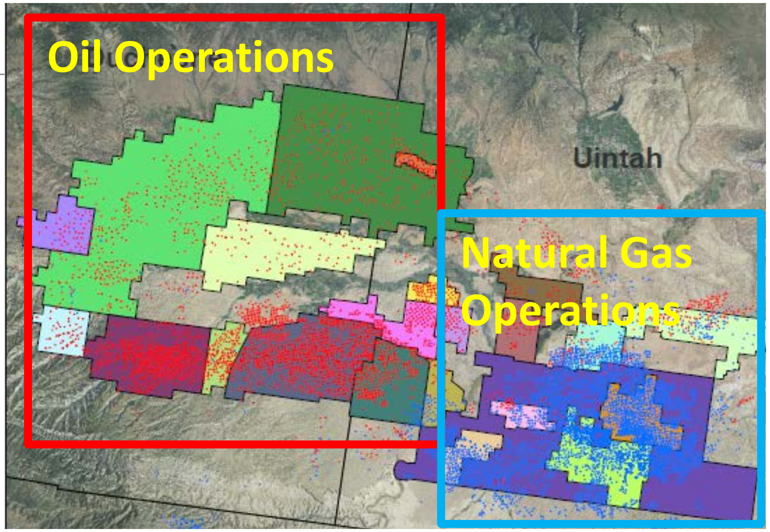
Motivation

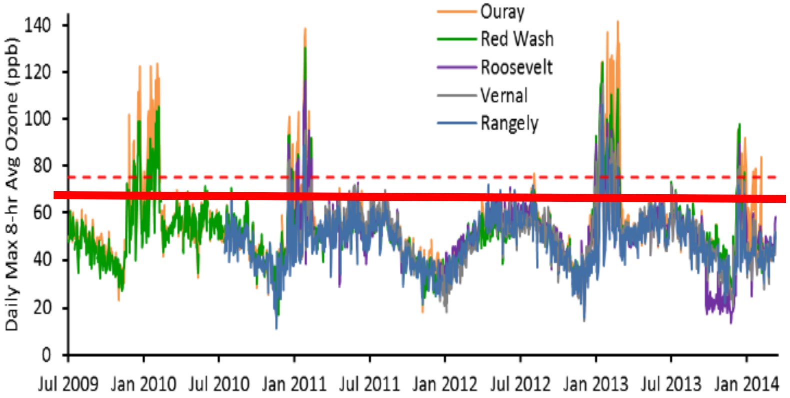
Extensive Oil and Gas Development: 24 O&G fields account for 90% of the 2013 O&G production in the Uinta Basin.

Complex Meteorology and Terrain: During winter season when the ground is covered by snow, these conditions create inversions and enhanced photolysis rates that result in ozone levels well above the National Ambient Air Quality Standards (NAAQS). First observed in Upper Green River Basin, WY by WDEQ in February 2005 (studied between 2007 and 2016).

Air Quality in 2013: Maximum 8-hour average ozone in Basin reached 142 ppb during the winter, 89% higher than the NAAQS. Ozone values exceeded NAAQS on 29 days and the ozone episodes ranged from 3 to 15 days in length.

Air Quality Prediction Capability: Air quality models are important for air quality management because they assist in identifying source contributions to air quality problems and designing effective strategies to reduce harmful air pollutants.





Objective and Approach

Environmentally responsible development of national energy assets requires:

- Well-developed emissions inventories, measurement techniques, and air quality modeling platforms.
- Accurate activity data, emission factors, and chemical speciation profiles for VOCs and NOx.

OBJECTIVE: Use CMAQ to help understand the causes of extreme winter ozone levels in areas with extensive oil and natural gas development.

- Focuses on the winter ozone issues in the Uinta Basin, Utah
- Performs model sensitivity tests to better understand factors important for predicting air quality impacts associated with oil and natural gas production:
    - Oil and Gas Emissions Inventory
    - Ozone Chemistry
    - Deposition
    - Meteorology

MANUSCRIPT: Evaluation of the Community Multiscale Air Quality Model for Simulating Winter Ozone Formation in the Uinta Basin, JGR, accepted for publication.

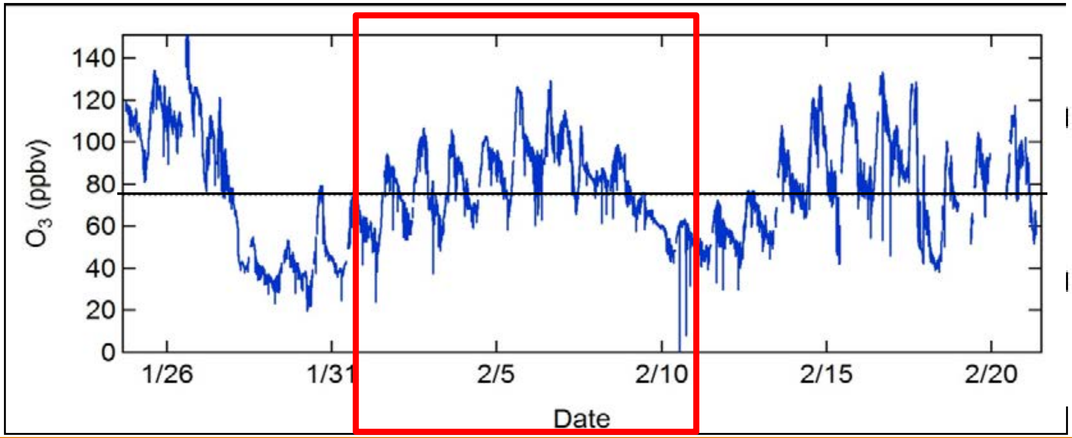
Episode Selection

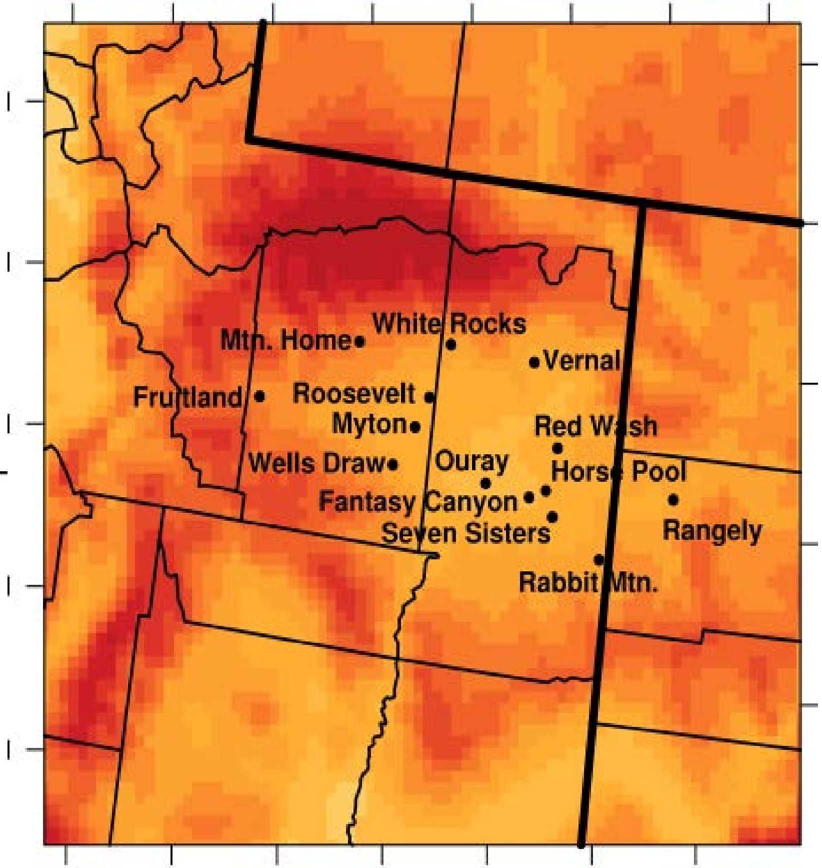
Uinta Basin Winter Ozone Study (UBWOS) 2013: Extensive field campaign from January to March 2013. Results from campaign provided information about meteorological conditions and atmospheric chemistry associated with winter ozone episodes in the Basin. This is important for model evaluation.

Select a period with winter ozone issues in Uinta Basin that has measurement data for model evaluation:
February 1st and February 10th of 2013

Participants with Instruments:

Types of Measurements: Aircraft, Balloon-borne, Tethered Ozonesondes, ground-based instruments





Air Quality Model Platform & Test Simulations

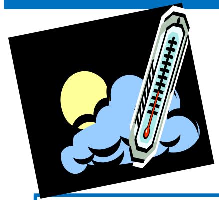
Weather Research and Forecasting Model (WRF-v3.6.1)

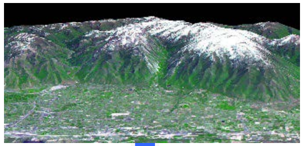
Topographic Information

Sparse Matrix Operator Kernel Emissions (SMOKE)

Motor Vehicle Emission Simulator (MOVES)

Biogenic Emissions Inventory System (BEIS)





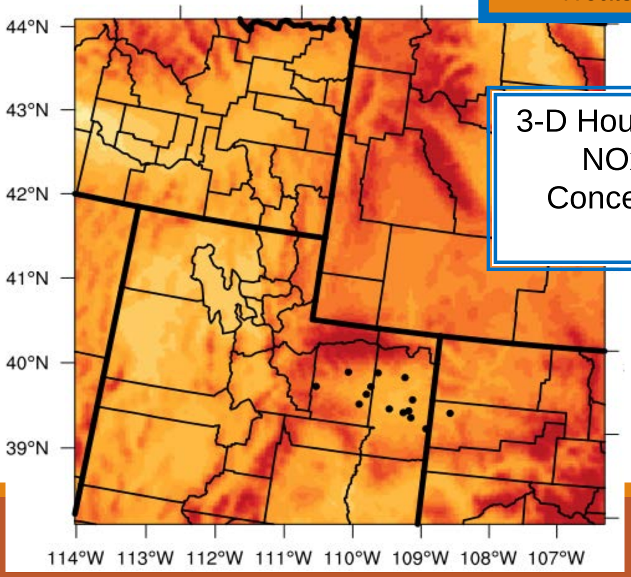
3-D Meteorological Information

Community Multiscale Air Quality Model (CMAQ – v5.0.2)

Treats dispersion, chemistry, and aerosol/cloud physics

3-D Emissions Information (2011 NEIv2)

3-D Hourly Predicted Ozone, Speciated NOx and VOCs, Methane, CO Concentrations and Dispersion and Chemistry Information



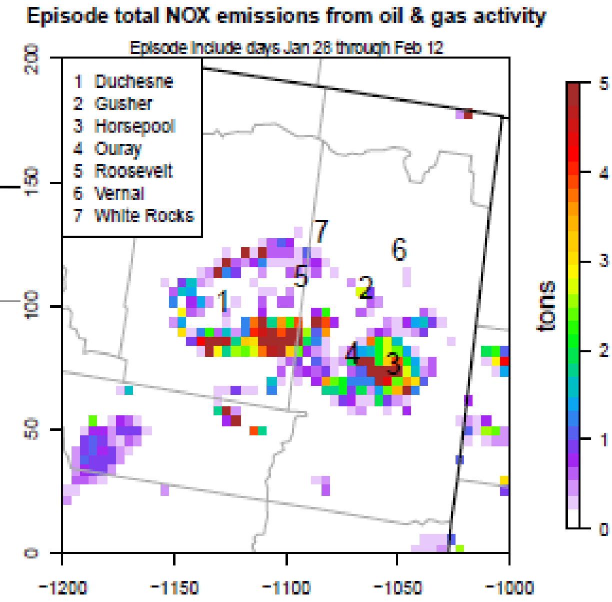
Performance of air quality models depend on accuracy of input parameters.

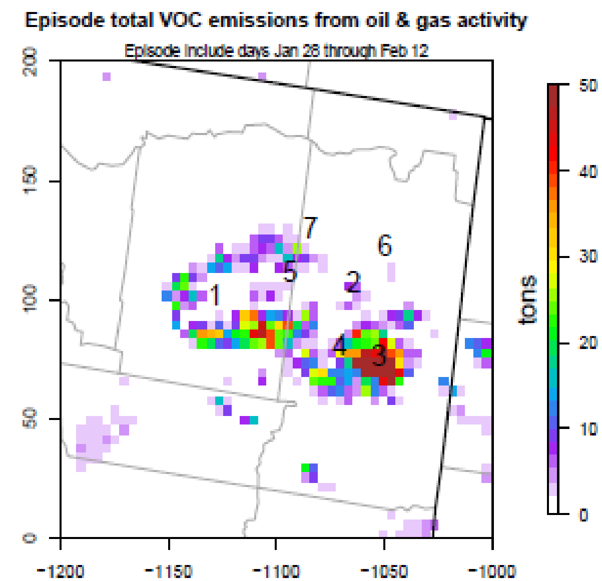
Conducted a number of simulations with:

- emission adjustments;
- deposition adjustments; or
- updated meteorological input.

Oil and Gas Emissions

Sector	NO_x Tons	VOC Tons	Top Processes
Non-point O&G	471.02	4010	Industrial Processes; Oil&Gas Exploration; Production
Point EGU	277.58	1.5	External Combustion Boilers; Electric Generation
Point O&G	89.06	12	Industrial Processes; Oil&Gas Production
On-road	83.54	38	Diesel; Combination short-haul trucks
Point Fire	26.65	500	Miscellaneous Area Sources
Non-Point	9.80	36	Stationary Source Fuel Combustion; Liquified Petroleum Gas; Natural Gas
Non-Road	9.65	48	Construction & Mining Equipment; Mobile Sources; Off-highway Vehicle Gasoline
Wood Combustion	0.58	6.3	Stationary Source Fuel Combustion; Residential





EPA Community Multiscale Air Quality Model (CMAQ)

Summary of Model Results

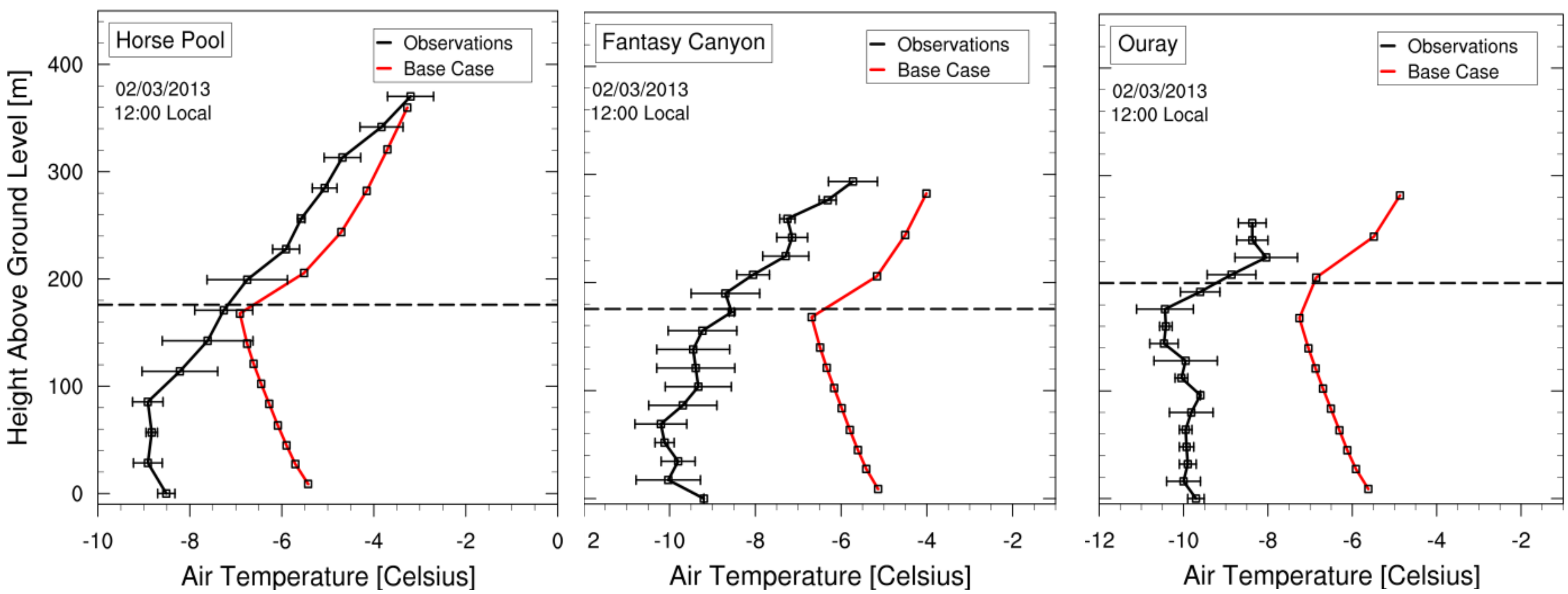
Standard CMAQ - Model Performance

Sensitivity to Meteorology

Sensitivity to VOC Emissions

Sensitivity to Deposition

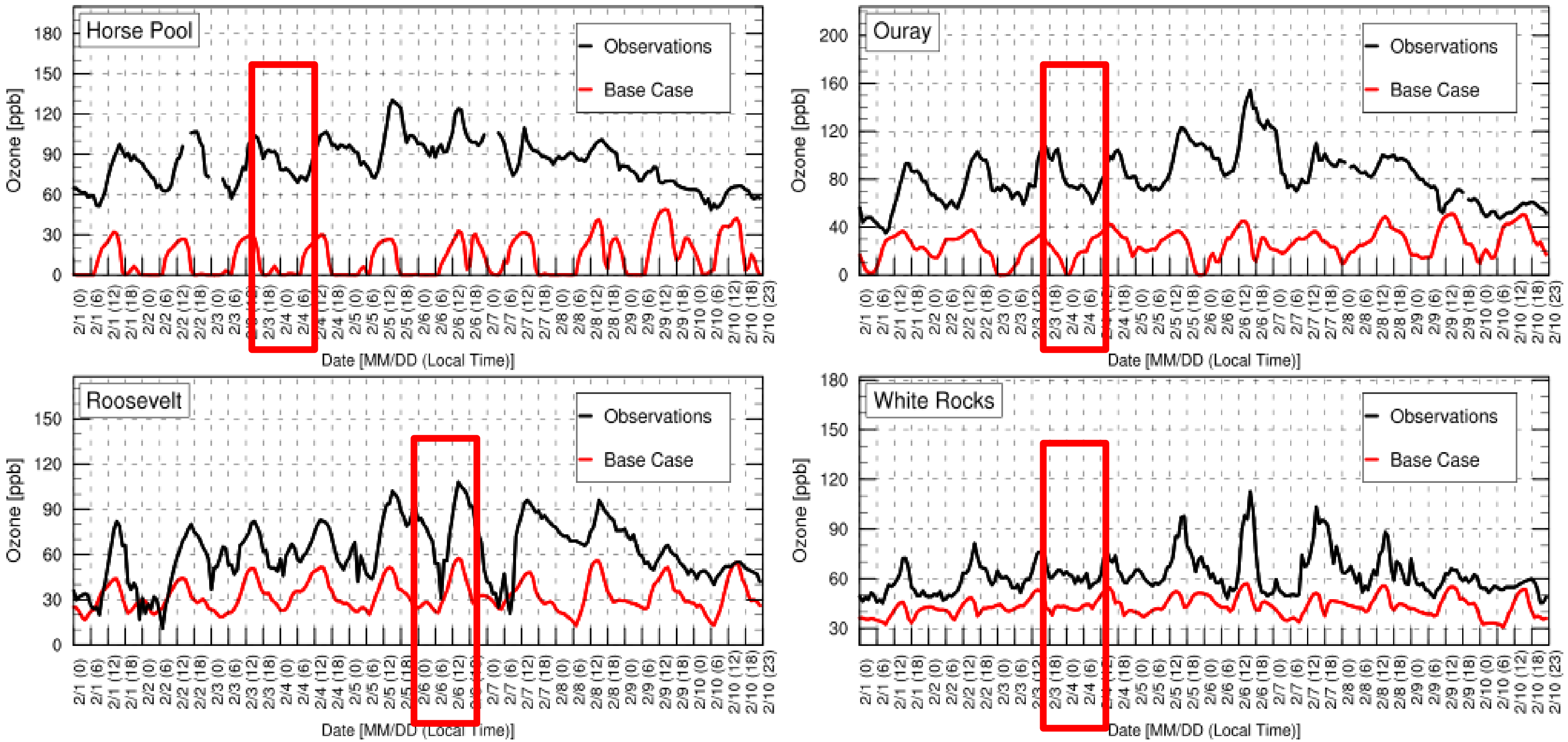
WRF Meteorological Performance



Vertical temperature gradients of WRF similar to observations, but model tends to over-estimate the temperature. Warmer temperatures suggests model has deeper boundary layer and greater vertical mixing.

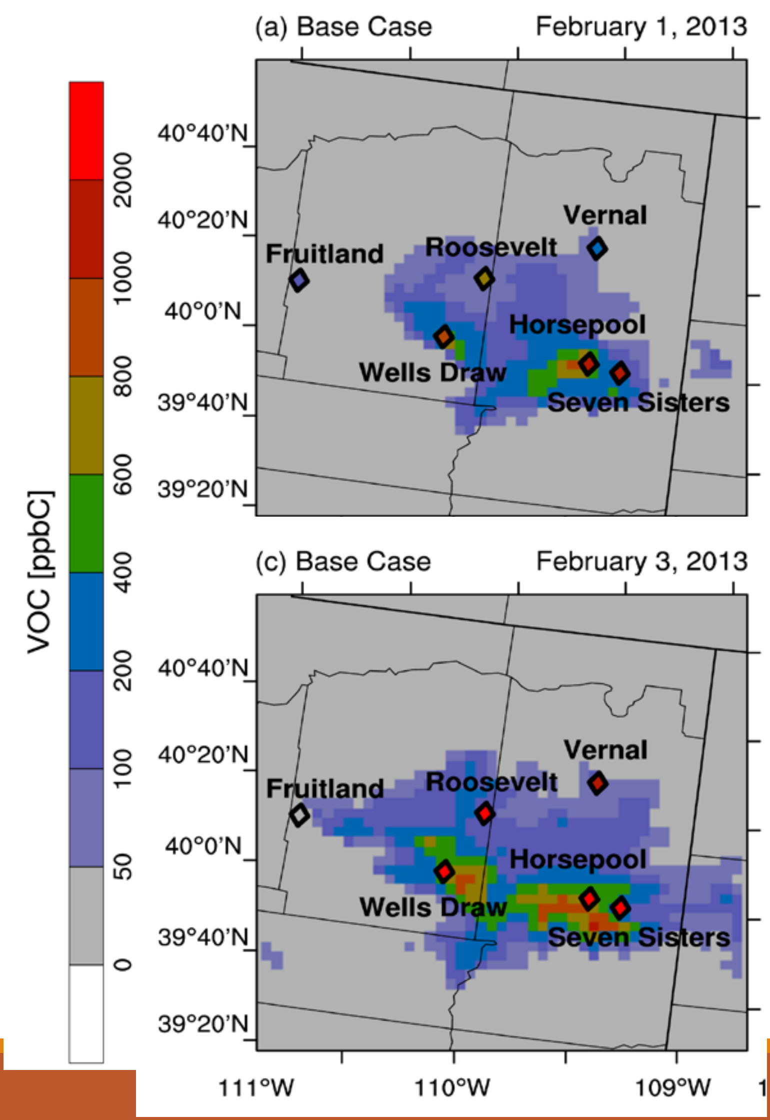
Could cause emissions at the surface to be dispersed into upper model layers, lowering predicted concentrations at ground-level.

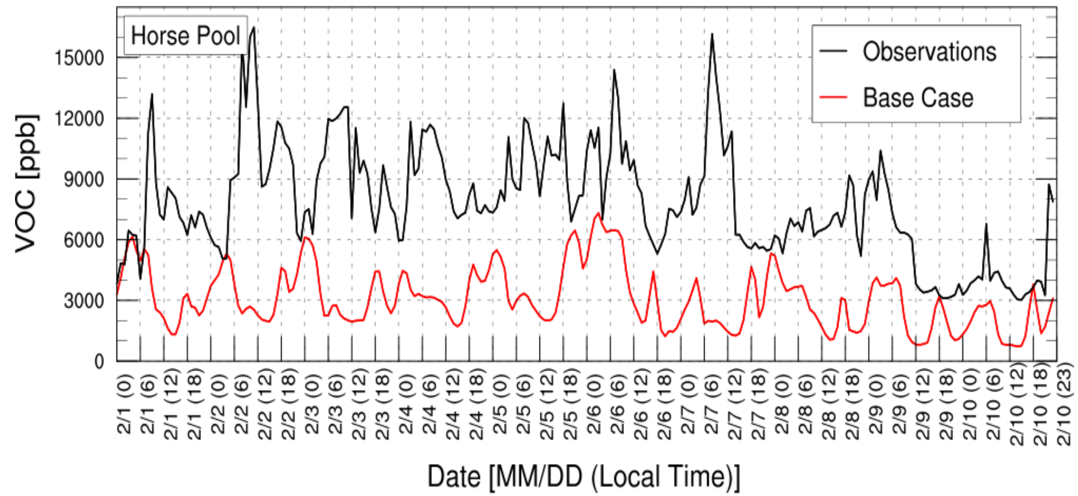
CMAQ Ozone Model Performance



Model captures diurnal variability in ozone at sites, but magnitude of model ozone is low and too much ozone is depleted at night.

CMAQ VOC Model Performance

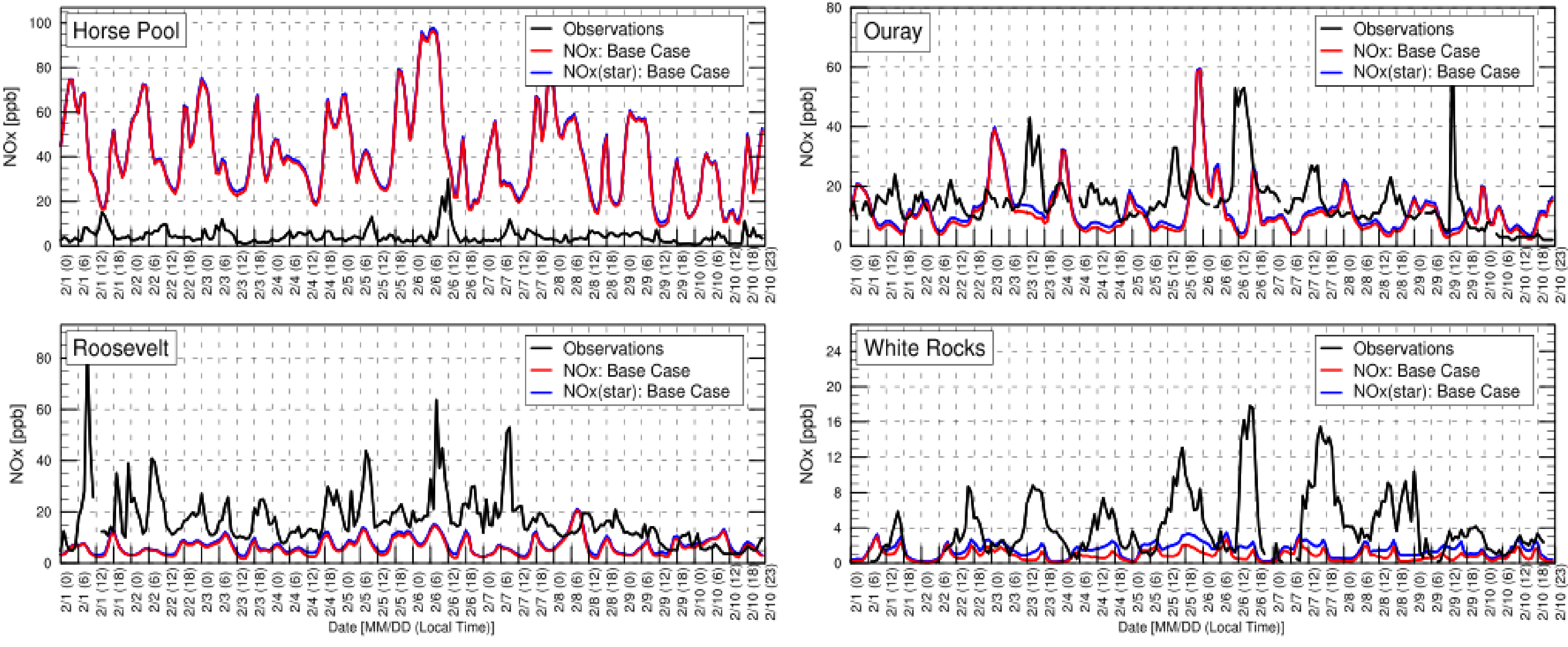




Model under-predicts the magnitude of VOCs at multiple monitoring sites within the Basin using the current version of the 2011 NEIv2 emissions inventory.

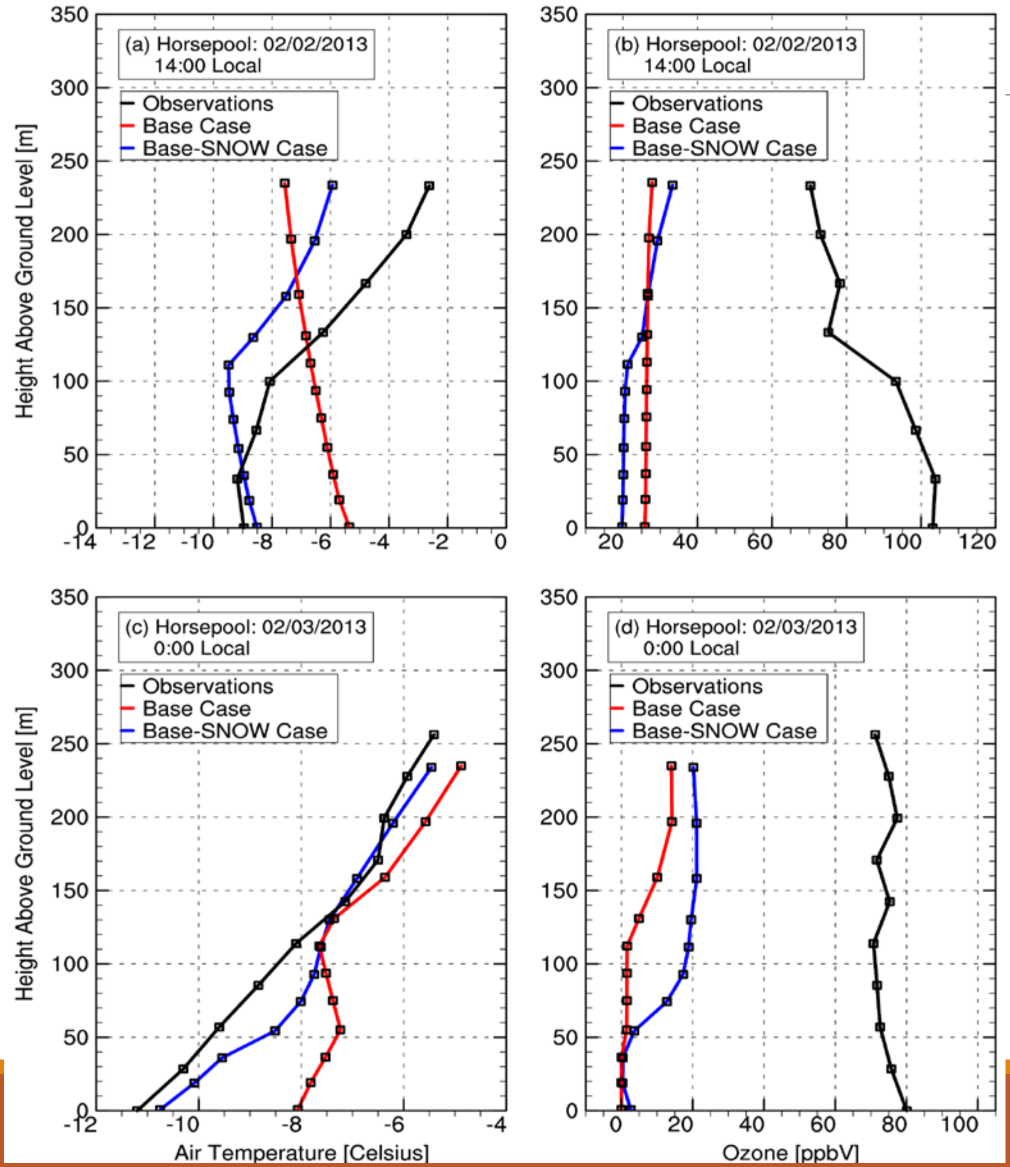
Lack VOC measurements within Basin to assist with model performance evaluations.

CMAQ NOx Model Performance



Magnitude of NOx over-predicted by model at Horsepool, and under-predicted at other sites. Differences among the observations at Horsepool and other sites may be an artifact of the measurement techniques (NOAA true NOx vs. AQS chemi-NOx).

WRF Sensitivity Test



To address general day-time warm bias, adjusted:

- Snow density: 250 kg m^{-3} to 50 kg m^{-3} to reflect western U.S.
- Snow albedo: 0.60 to 0.80

While adjustments improve vertical profiles of air temperature, the vertical profiles of ozone seldom resulted in improvements.

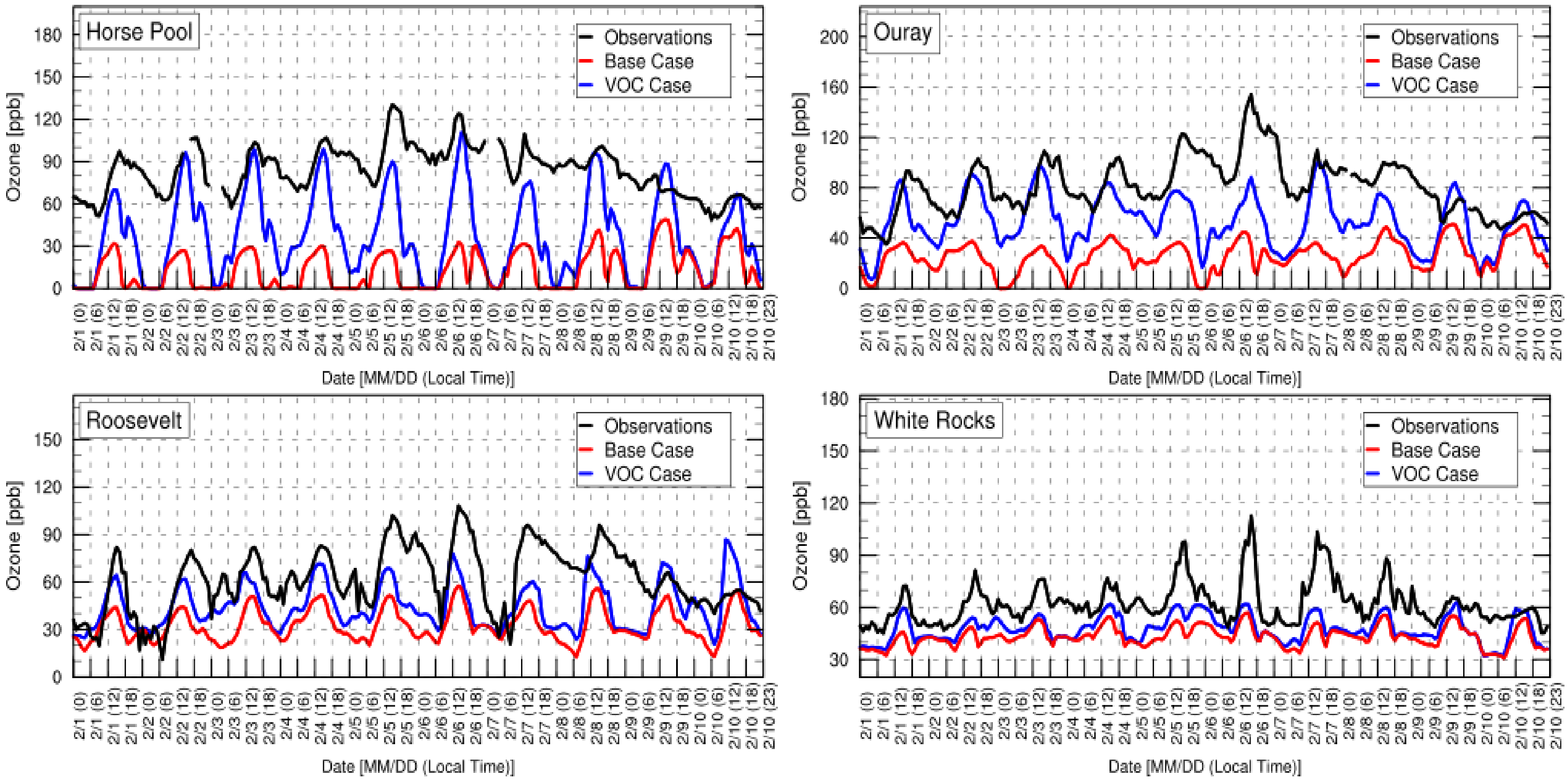
Results suggest that the 2011 NEIv2 O&G emissions is likely the major contributor to negative bias in the predicted VOC and NOx at the surface.

CMAQ VOC Sensitivity Test

Modeled Species	Description	Baseline Total	Adjusted Total	Adjustment Factor	Scaling Species
		Episode Total Tons			
CH4	Methane	5938	17,817	3.0	CH4
ALD2	Acetaldehyde	0.01	0.2	16.4	PAR*3.5
ALDX	C3 + aldehydes	0.004	0.007	1.6	PAR*3.5
ETH	Ethene	0.28	3	9.8	PAR*3.5
ETHA	Ethane	708	1417	2.0	ETHA
ETOH	Ethanol	0.004	0.02	5.3	PAR*3.5
FORM	Formaldehyde	0.8	15	19.6	PAR*3.5
IOLE	R-HC=CH-R	0.2	0.2	1.0	IOLE
MEOH	Methanol	1.1	217	200.0	MEOH
OLE	Alkenes	0.8	3	3.5	PAR*3.5
PAR	C-C bond	2078	7273	3.5	PAR
TOL	Toluene and similar	72	649	9.0	TOL
UNR	Unreactive	275	275	1.0	UNR
XYL	Xylene and similar	44	654	15.0	XYL
BENZENE	Benzene	8	51	6.0	BENZENE

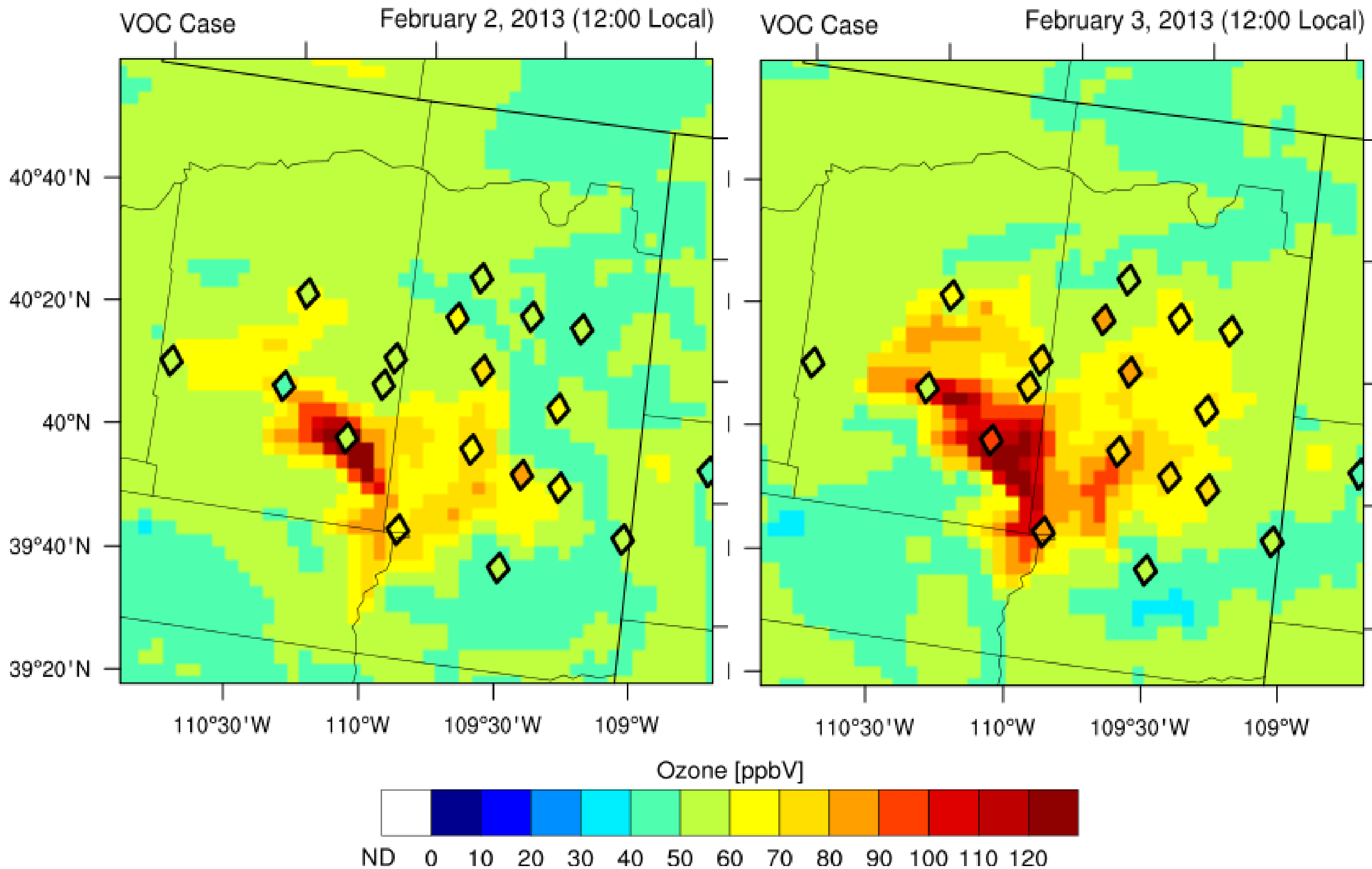
VOC emission adjustments determined by matching model results to observed mixing ratios at Horsepool. PAR used to scale species without reported emissions. These factors were applied every day/time and across the domain.

Results – VOC Sensitivity Test



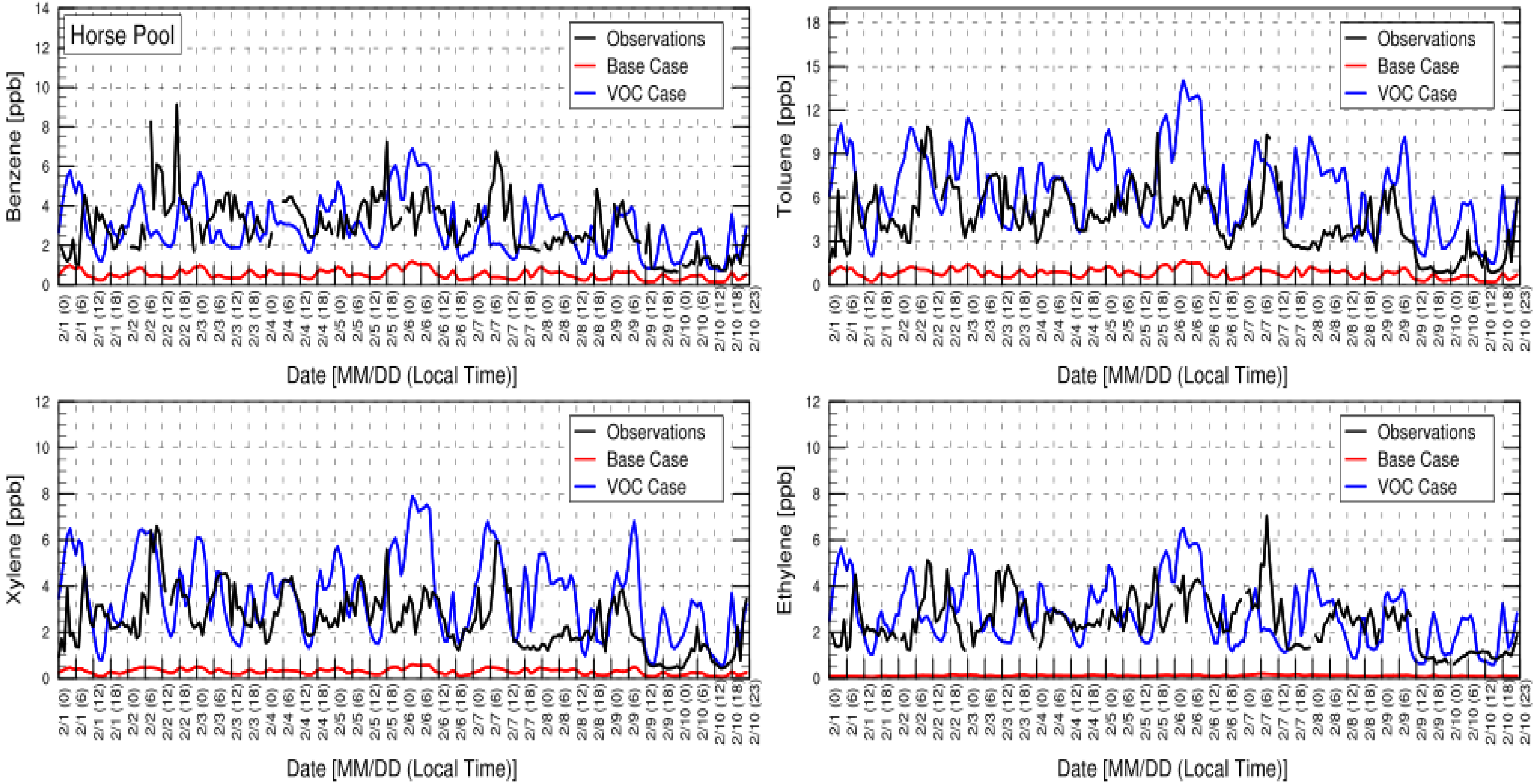
Magnitude of model ozone significantly increases during the day as a result of adjusting the VOC oil and gas emissions. Model ozone continues to be biased low during the night.

Results – VOC Sensitivity Test



Adjusting the VOC O&G emissions improves model performance across basin for ozone.

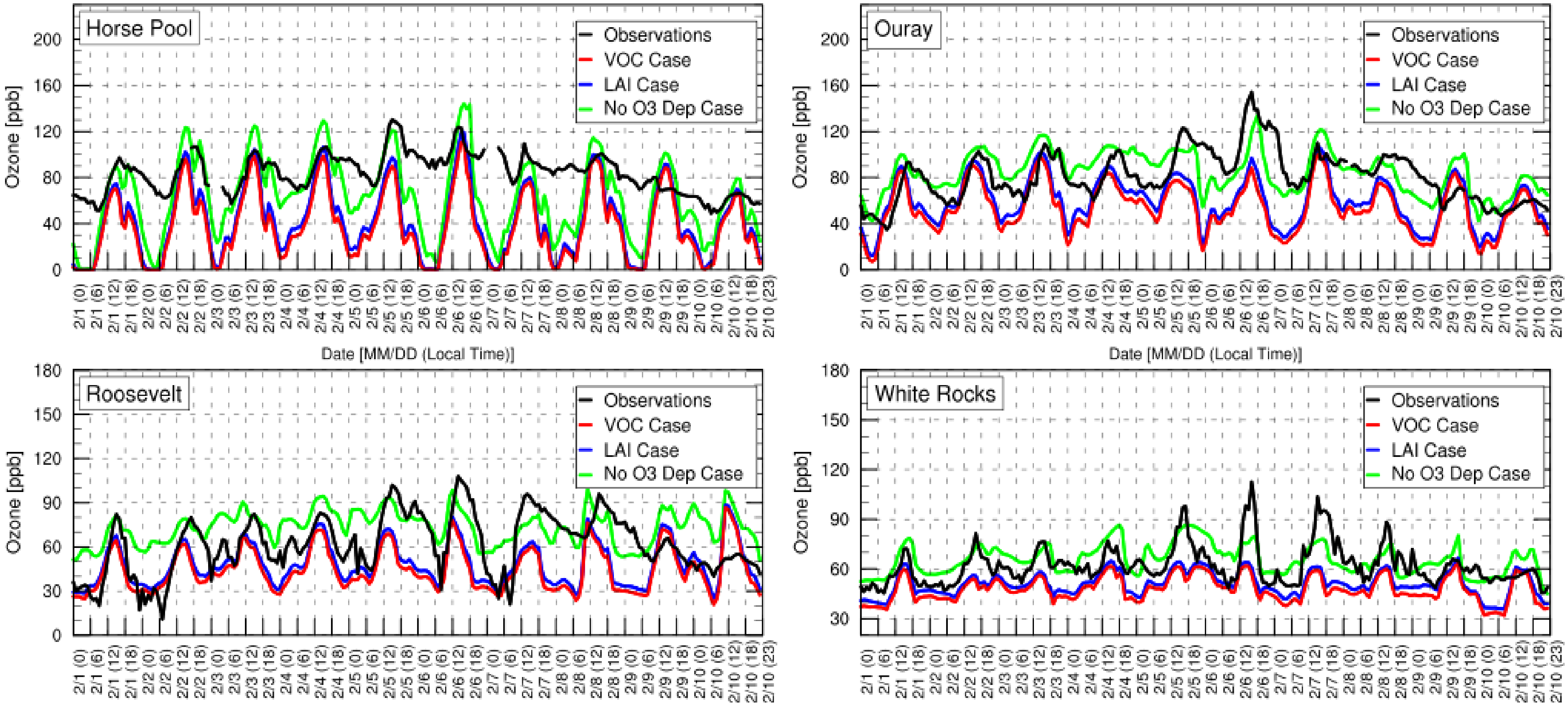
Results – VOC Sensitivity Test



Adjusting VOC O&G emissions also improves model performance for speciated VOCs.

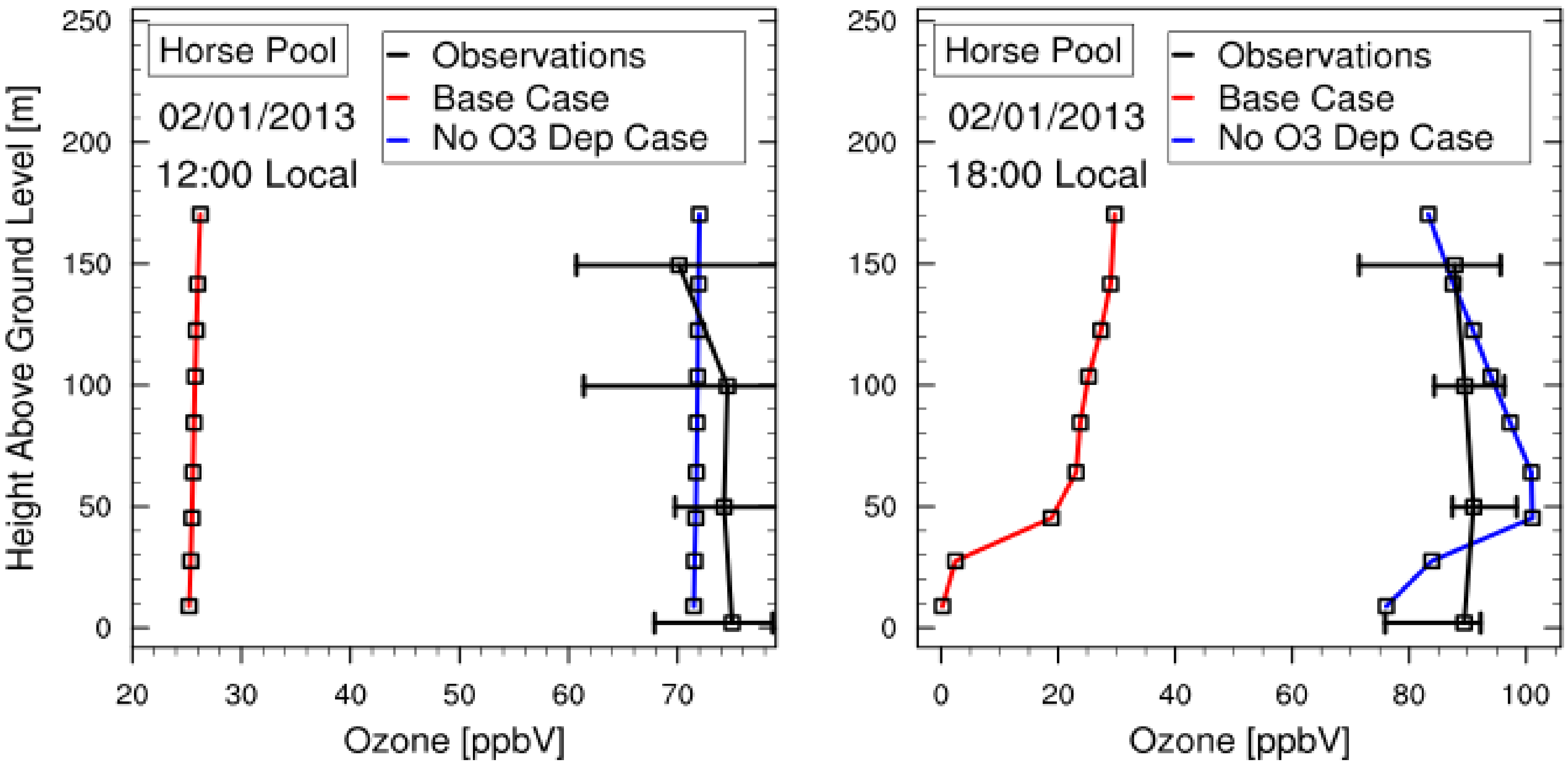
Additional efforts are needed to investigate the 2011 NEIv2 O&G emissions.

Results – Deposition Sensitivity Tests



Measured daytime O_3 deposition velocity at Horsepool: -0.071 – 0.079 cm s^{-1}. Model deposition velocity: 0 – 0.21 cm s^{-1}. Tests: (1) Grids with scrub/barren vegetation and snow-covered set to 0.001; (2) zero O_3 dry deposition. Magnitude of nighttime model ozone significantly increases.

Results – Deposition Sensitivity Tests



Adjustments in deposition velocities also improves model vertical profiles.

Additional work is needed to investigate CMAQ's treatment of deposition over snow.

Summary and Key Findings

A number of WRF and CMAQ simulations were performed to understand sensitivity to uncertainty in emissions, chemistry, transport, and meteorology. Key Findings:

- Baseline model had a large negative bias when compared to ozone, VOC, and NOx measurements across the Basin.
- Increases to VOC O&G emissions resulted in ozone predictions closer to observations during day-time.
- Nighttime ozone improved when deposition velocities were set to zero.
- Warmer temperatures predicted by the model suggests model has deeper boundary layer and greater vertical mixing. Potential to contribute to negative bias in the predicted VOC and NOx concentrations at the surface because the emissions are being diluted in a deeper mixed layer. However, the meteorology does not appear to be the major contributor to the overall under-predictions.

Results suggest significant uncertainty in 2011 NEIv2 O&G emissions for the Uinta Basin and deposition algorithms within the model over snow. Additional measurement data are needed for model performance evaluation.

Future Work

- **Due to the uncertainty in the VOC and NOx emissions, model performed poorly for ozone in the Uinta Basin. Additional studies are needed to improve O&G emission inventories.**

- **Continue collaboration between Region 8, OAQPS, and ORD to further investigate parameters influencing model results to improve model performance:**
  - Emissions: Improve oil and gas emissions inventories.
  - Deposition: Improve deposition velocities to snow for all species and evaluate snow as a reservoir and possible source of heterogeneous chemistry of VOC and NOx.
  - Meteorology: Parameterizations used to represent boundary layers and ice fog processes in numerical models to obtain improved cold air pool simulations.
  - Measurements: Plan for new or additional NOx and VOC measurements to better understand winter photochemistry and deposition processes.
  - Expand methodologies and tools to other oil and gas producing regions and air quality applications.