Modeling of air quality over U.S. oil and natural gas producing regions with WRF-Chem

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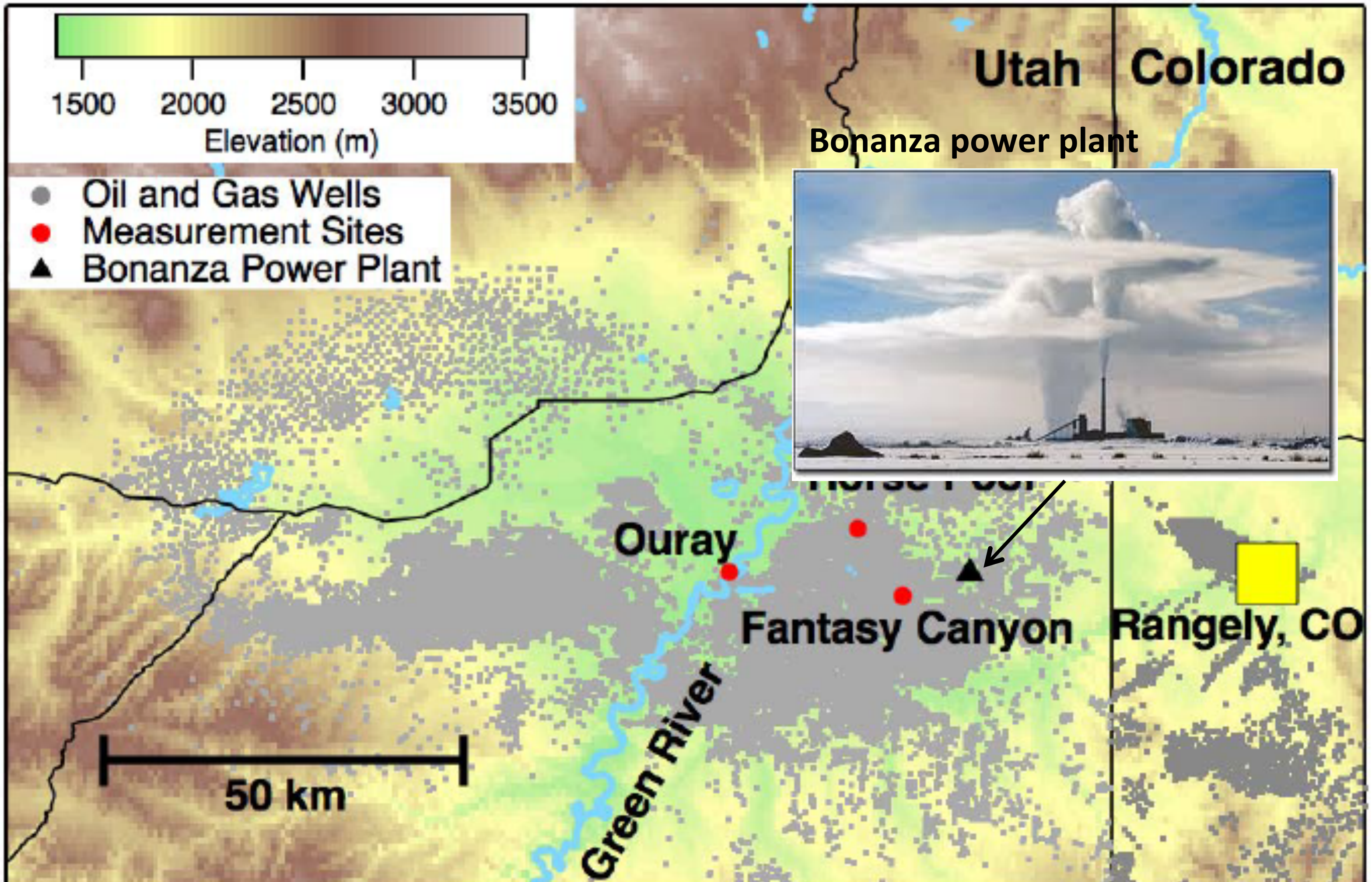
WRF users' workshop
Boulder, June 18, 2015

Permian drilling activities 6 April Photographer: C. Brock

Introduction

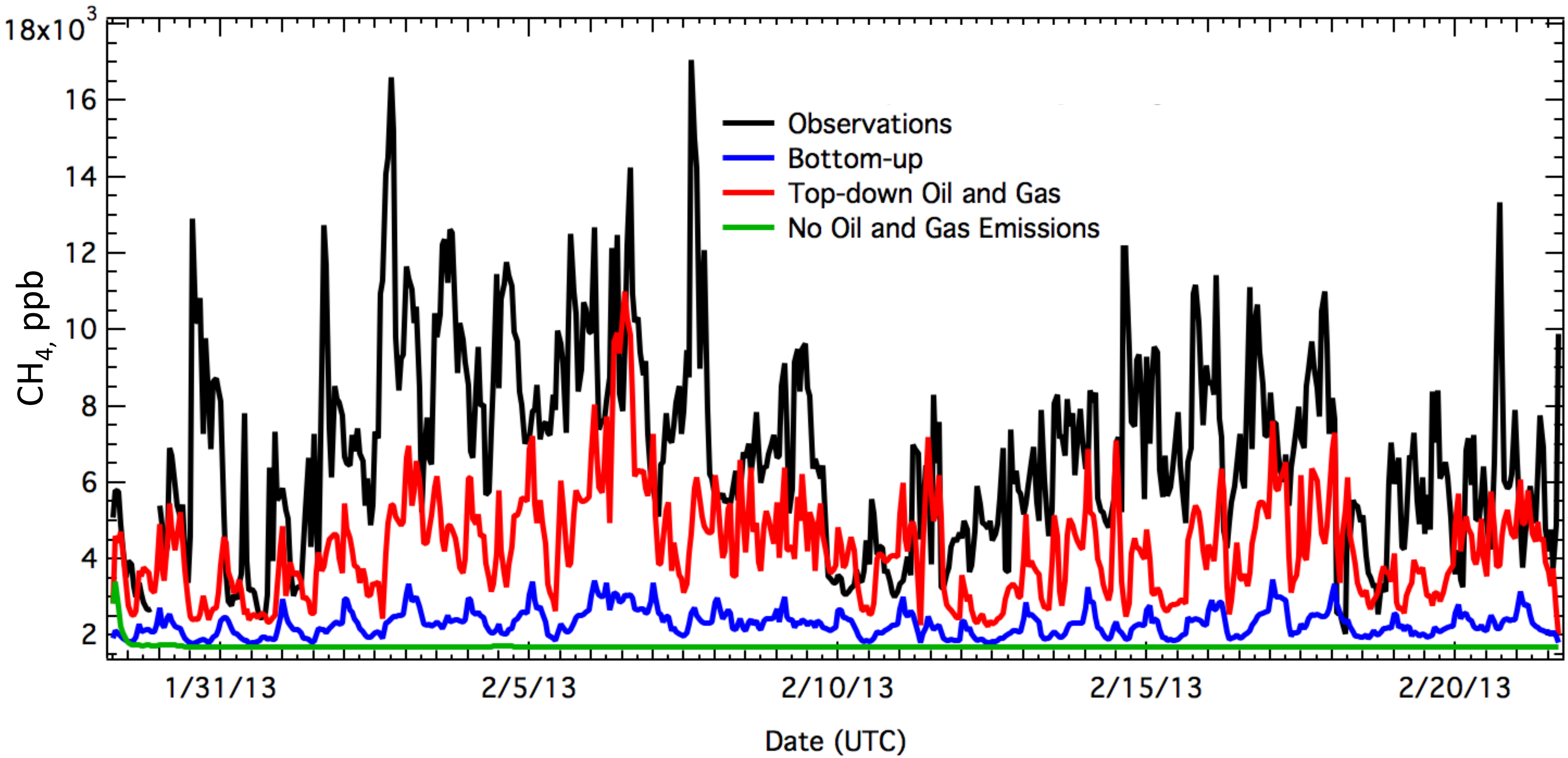
- During some winters over rural areas with high oil/gas production in Wyoming and Utah high ozone episodes were observed (*Schnell et al., 2009; Oltmans et al., 2014).*
- It is important to model the high wintertime ozone events by air quality models in order to understand, predict and mitigate wintertime ozone pollution events.
- Air quality models were unable to predict or reproduce the high wintertime ozone episodes in the US observed in recent years.
- Main challenges for modeling such pollution episodes: complex terrain and meteorology, snow effect on chemistry, deposition and photolysis fluxes and poorly constrained oil and natural gas emissions.
- We targeted the wintertime ozone pollution events by leveraging off the NOAA's measurements and the WRF-Chem capabilities.

Topography of the Uinta Basin, Utah



The region is sparsely populated (~50,000 people). The urban VOC and NO_x emissions are not high.

Observed and modeled methane time series at the surface site in 2013



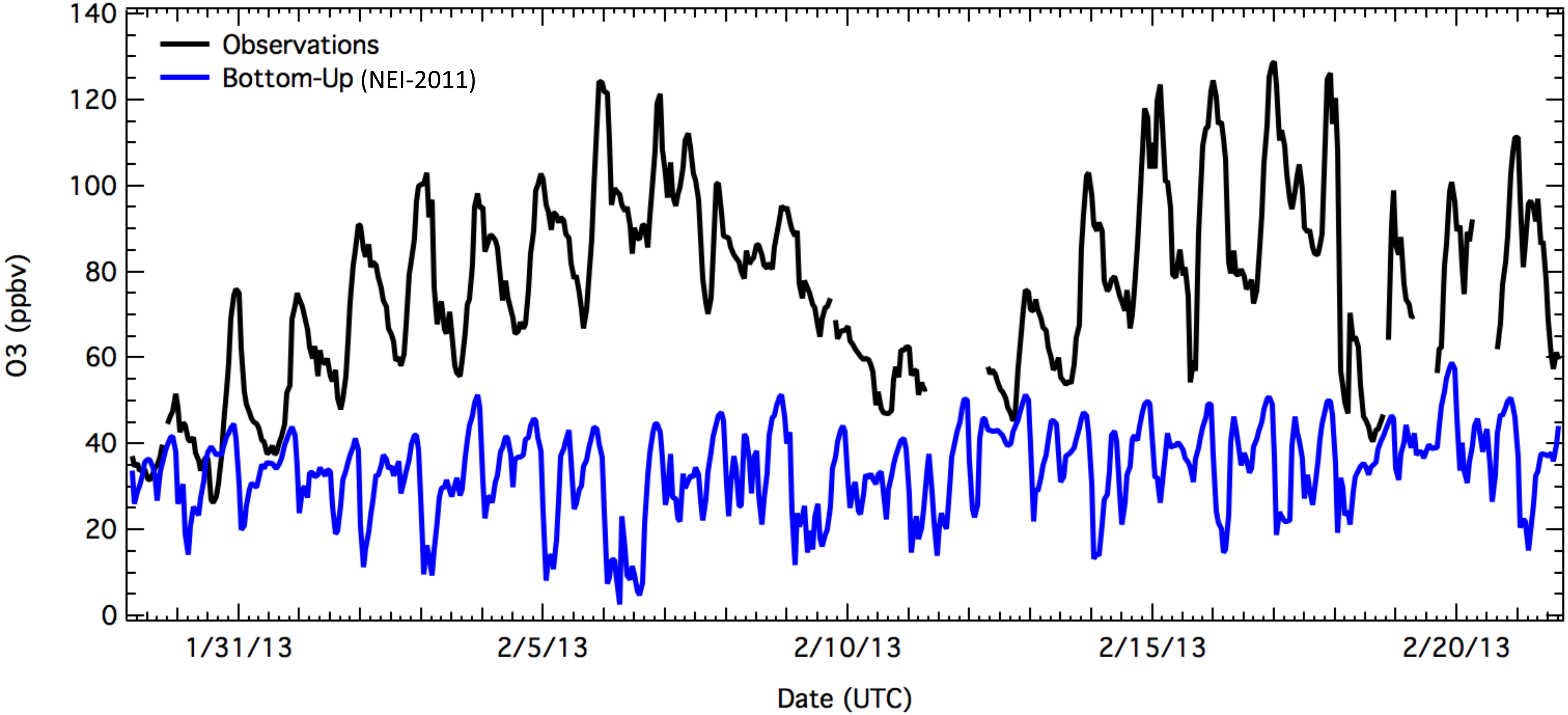
The simulated methane mixing ratios using the top-down emission estimates (Karion et al., 2013, based on one day aircraft flight measurements) show a better agreement with the observation compared to the bottom-up inventory.

First verification of a top-down emission estimate of methane for a shale basin using a 3D model!

Observed and modeled ozone time series at the surface site during winter of 2013

Multi-day buildup of surface O_3 during the stagnation episodes

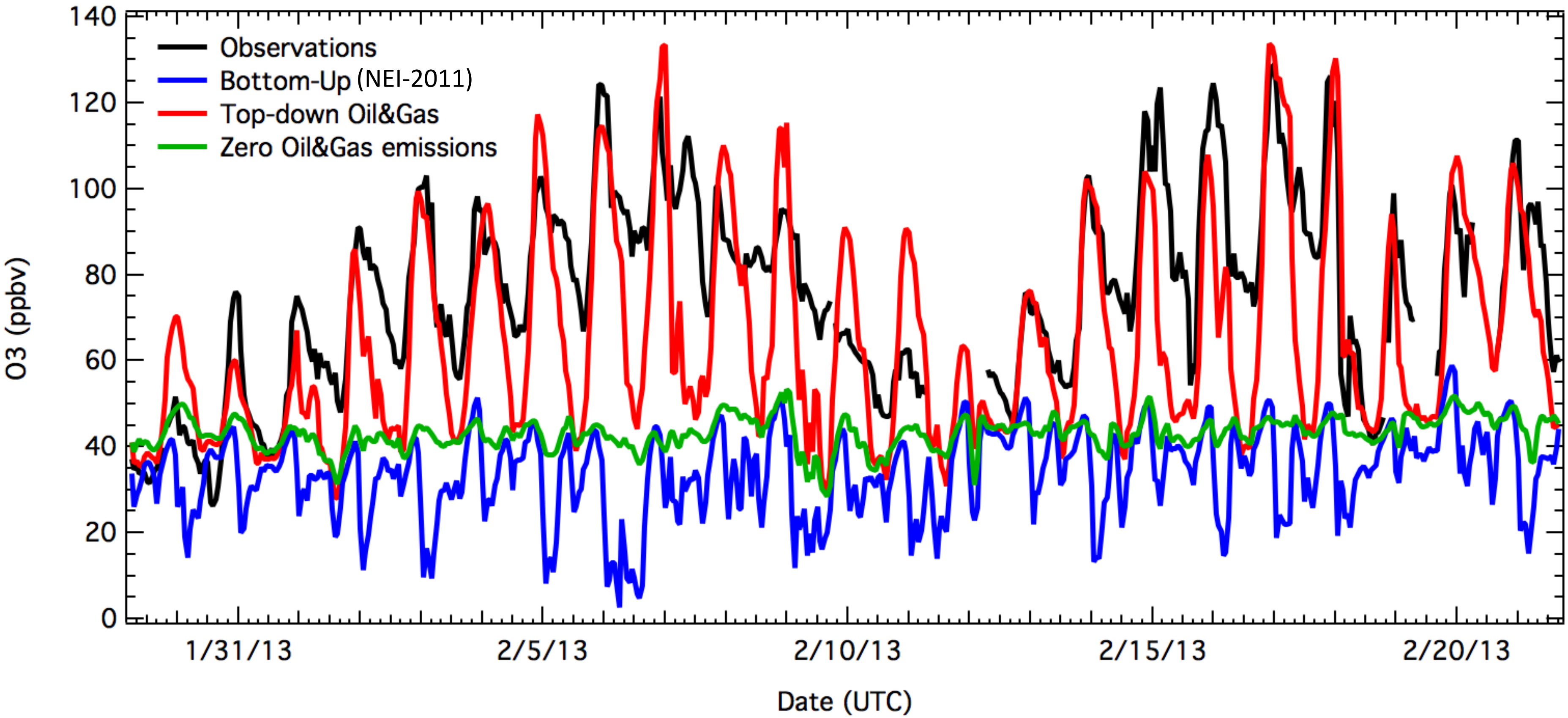
The model using the EPA emissions fail to reproduce the observed high O_3 levels!



Ahmadov et al. (2015), ACP

Observed and modeled ozone time series at the surface site during winter of 2013

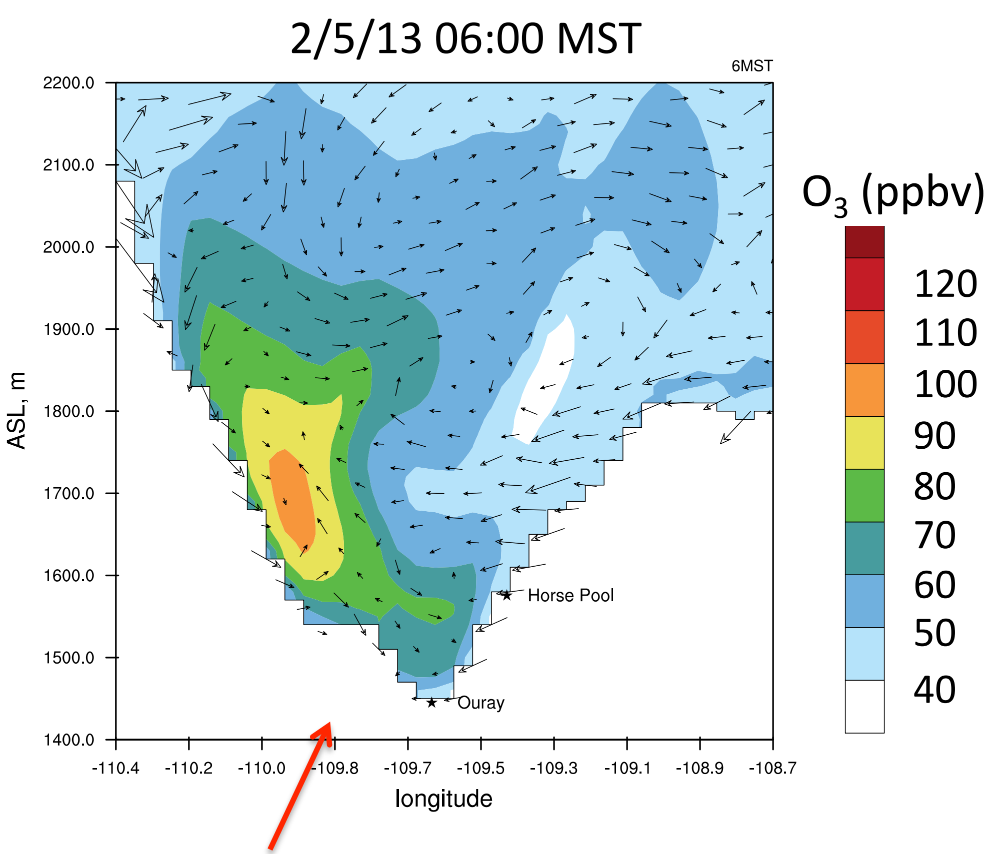
Only the top-down emission case can explain the high ozone levels!
The high ozone in the Uinta Basin is driven mostly by the oil/gas emissions!

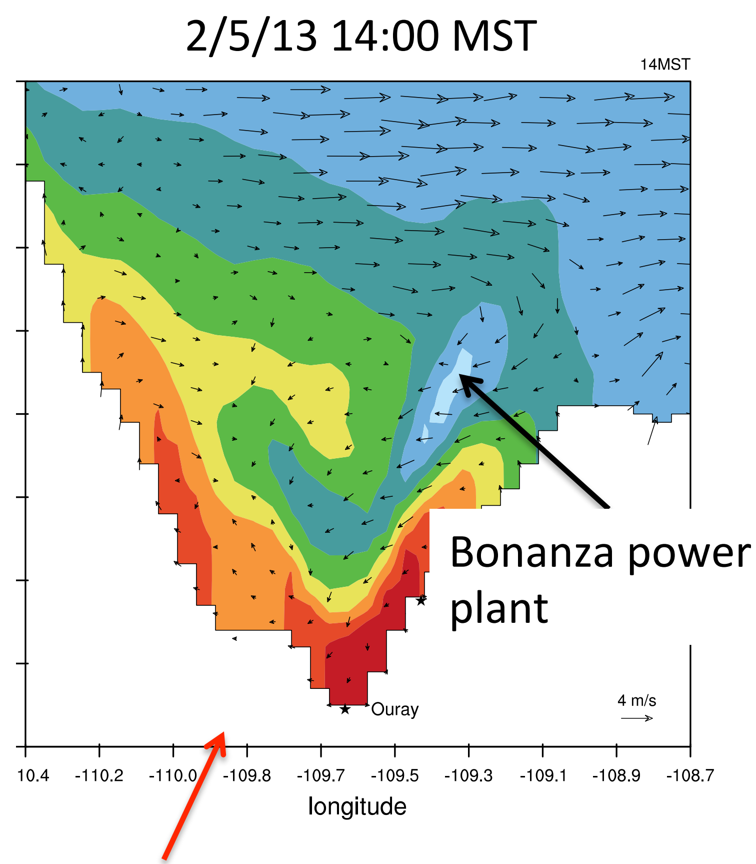


Several modifications are implemented in the WRF-Chem model for better handling the wintertime conditions affecting the photochemistry and dry deposition.

Ahmadov et al. (2015), ACP

West-East cross-section through the Uinta Basin





<u>Nighttime and Early Morning</u>

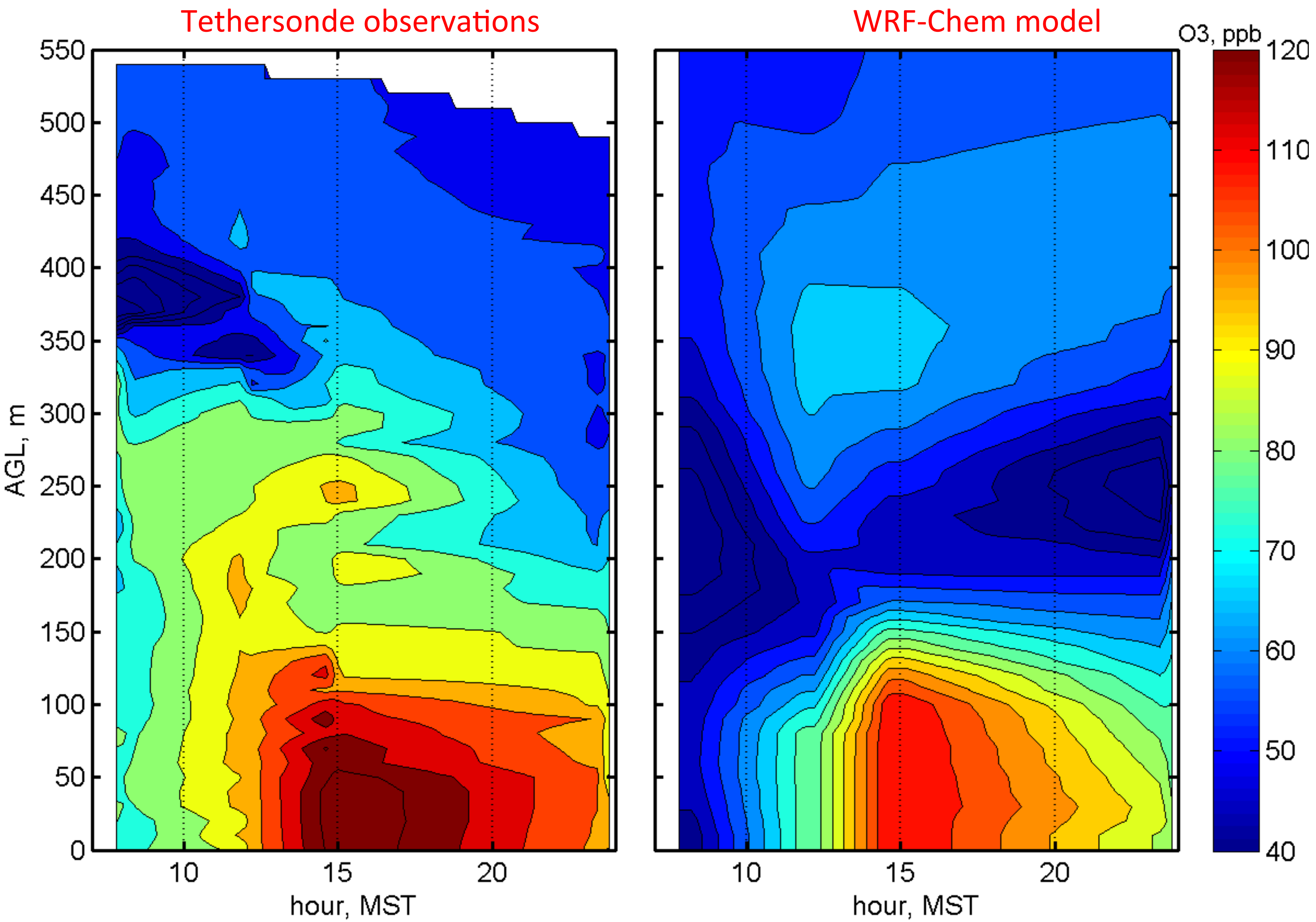
- Strong drainage flow
- Complicated circulation within Basin
- O_3 from previous day trapped

<u>Daytime</u>

- Light winds within Basin
- Low Mixing Heights
- Significant O_3 buildup in shallow layers

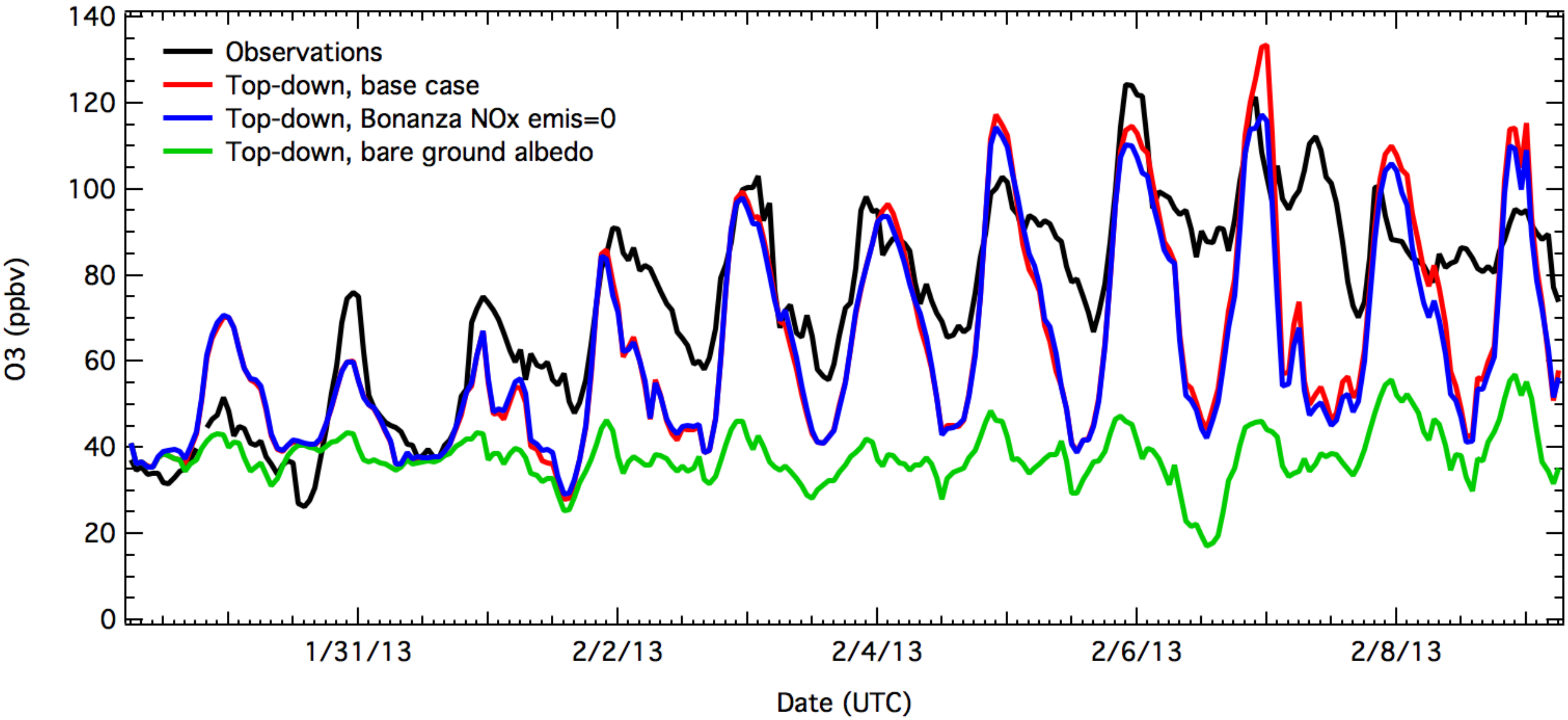
Ahmadov et al., ACP, 2015

Ozone distribution over the surface site on February 5th, 2013



Is ozone photochemistry sensitive to the Bonanza power plant emissions and snow albedo?

Bonanza power plant: No
Snow albedo: Yes



Importance of the snow albedo effect on the photolysis fluxes!
The Bonanza power plant emissions do not mix within the boundary layer (importance of the vertical mixing in the WRF-Chem model)

Highlights of the WRF-Chem perturbation/sensitivity analysis

Physical Processes - Perturbation Case	Impact on model O_3 from oil/gas
Bare ground surface albedo (no snow)	104%
Bare ground O_3 surface deposition	48%

Snow is essential for high O_3

NO_x Emission Perturbation Case	Impact
Top-Down Oil&Gas NOx Emission Reduced 30%	1%
Top-Down Oil&Gas NOx Emission Reduced 67%	14%
Top-Down Oil&Gas NOx Emission Reduced 100%	45%

High O_3 events are insensitive to NO_x reductions

VOC Emission Perturbation Case	Impact
Top-Down Oil&Gas VOC emis. Reduced 30%	33%
>C-2 Alkane VOC emis. set to zero	44%
Aromatic VOC emis. set to zero	37%

Top-down Aromatic/(>C-2 alkane) flux ratio = 0.10

O_3 is VOC limited

Aromatics have a disproportionate influence

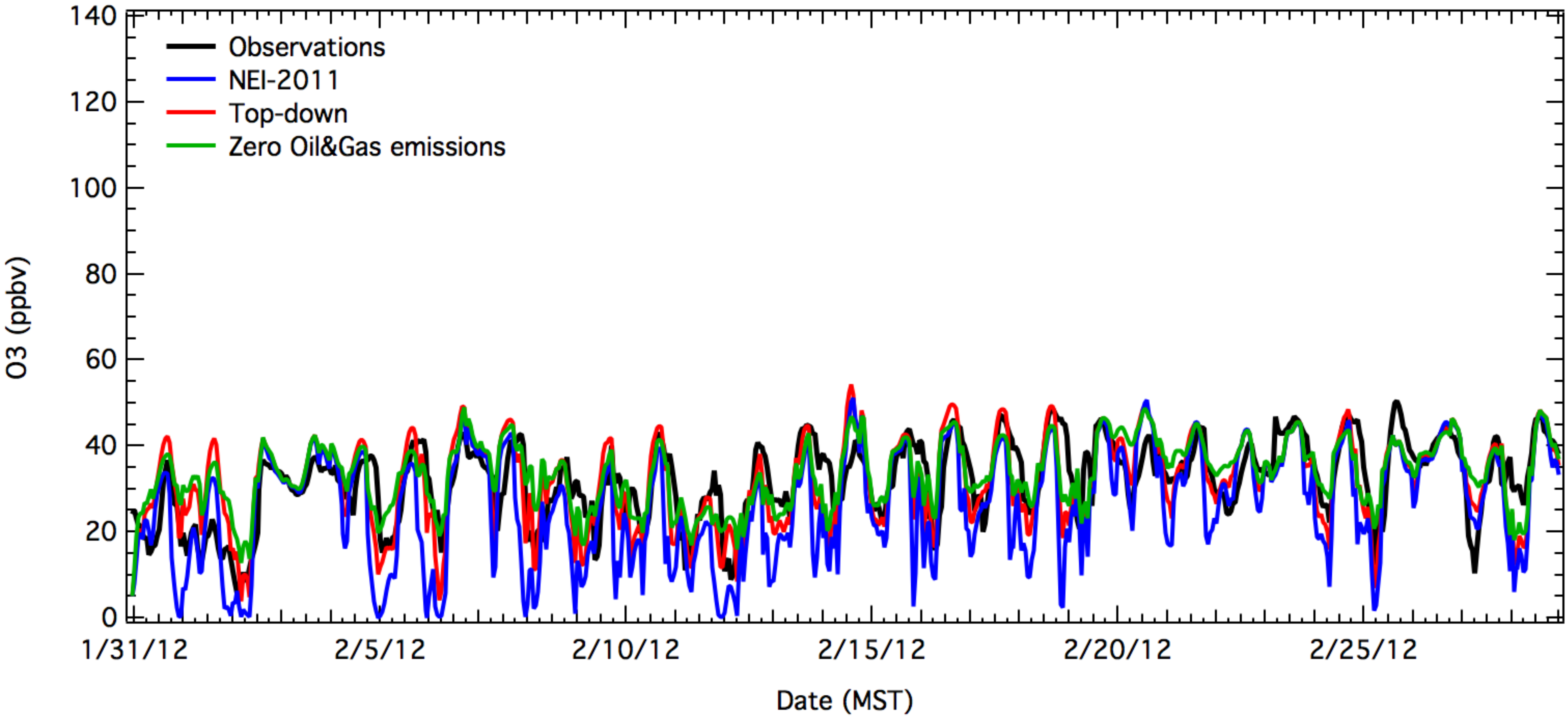
Ahmadov et al., ACP, 2015

Summary

- ✓ The emission inventories (CH_4, VOCs and NO_x) for the oil/gas sector can be significantly improved by using the top-down emission estimates.
- ✓ The WRF-Chem model (modified for wintertime conditions) is able to simulate high O_3 episodes in winter of 2013 using the top-down emission estimates, but not the bottom-up (NEI-2011) inventory.
- ✓ High ozone in the Uinta Basin are primarily caused by the very high VOC versus NO_x emissions from the oil/gas sector, persistent stagnation episodes and high surface albedo and reduced deposition effect due to snow cover.

Thank you for your attention!

Observed and modeled ozone time series at the Horsepool site, 2012

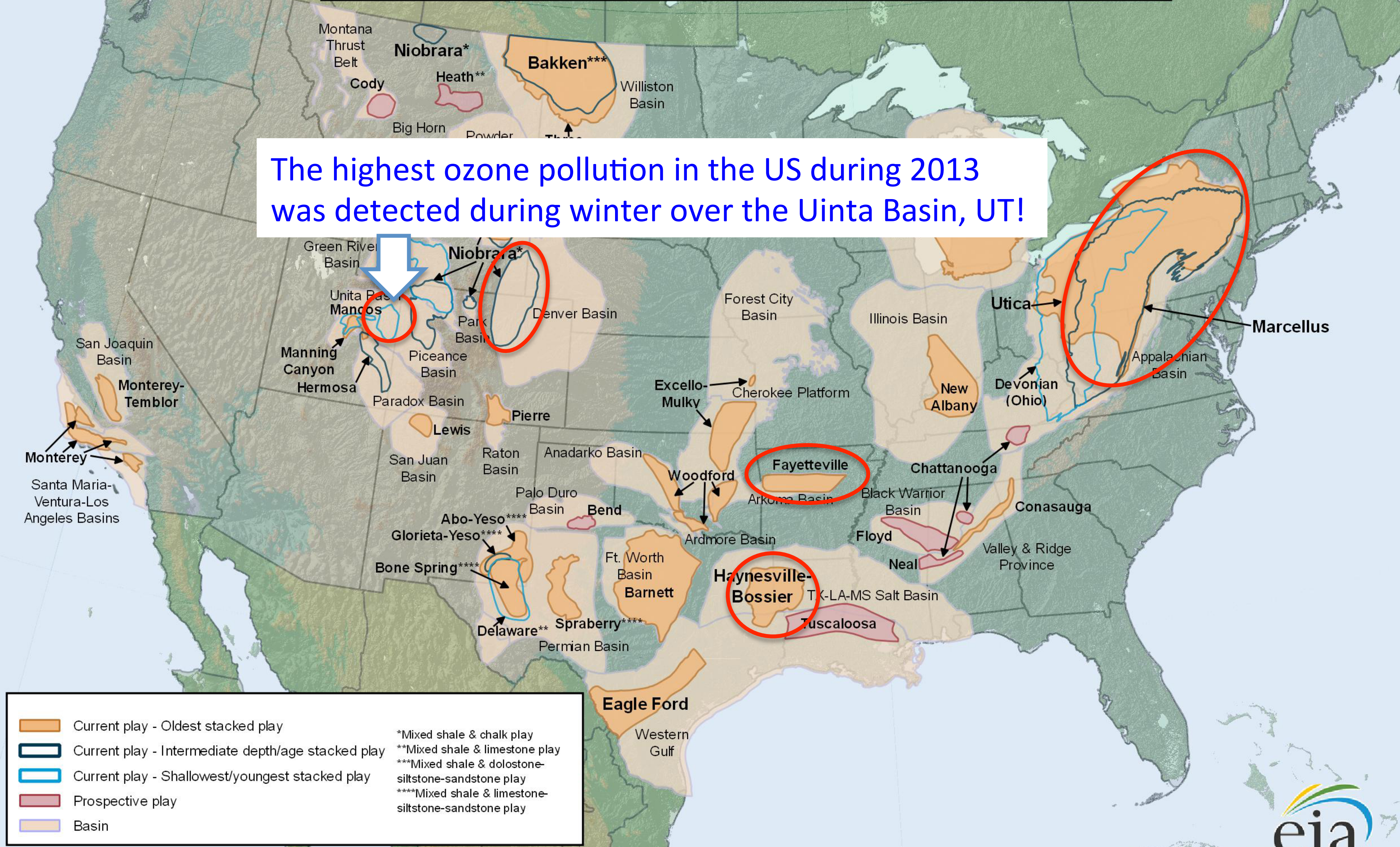


The same model settings and emissions for the 2012 and 2013 cases were used!

Ahmadov et al. (2014), ACPD

Lower 48 states shale plays

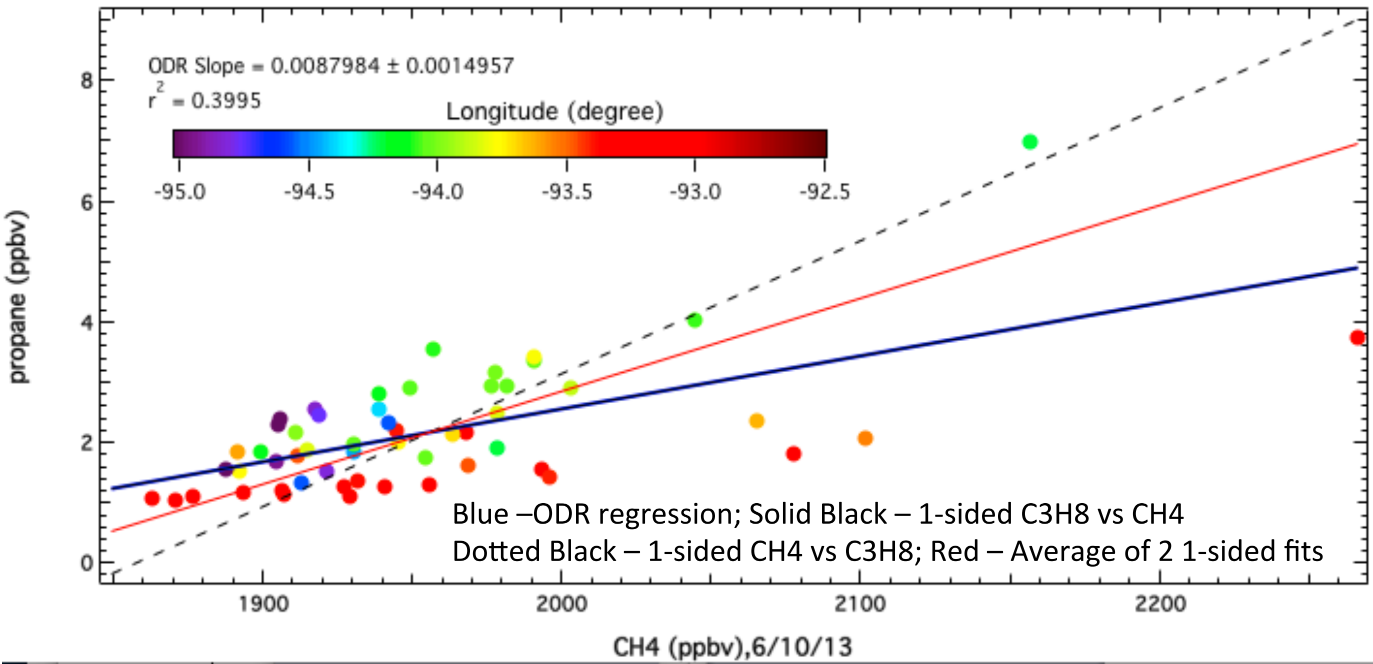
The highest ozone pollution in the US during 2013 was detected during winter over the Uinta Basin, UT!



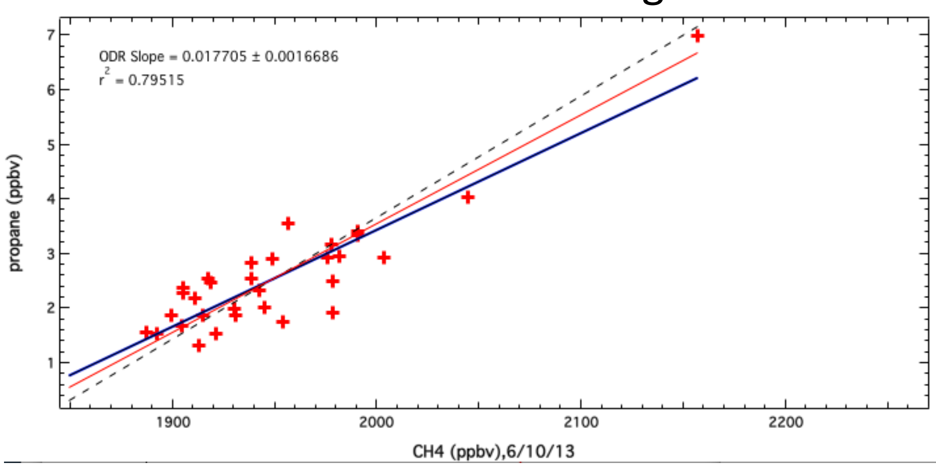
Source: U.S. Energy Information Administration based on data from various published studies.
Updated: January 8, 2015

Example of SENEX-2013 regressions: C_3H_8 versus CH_4

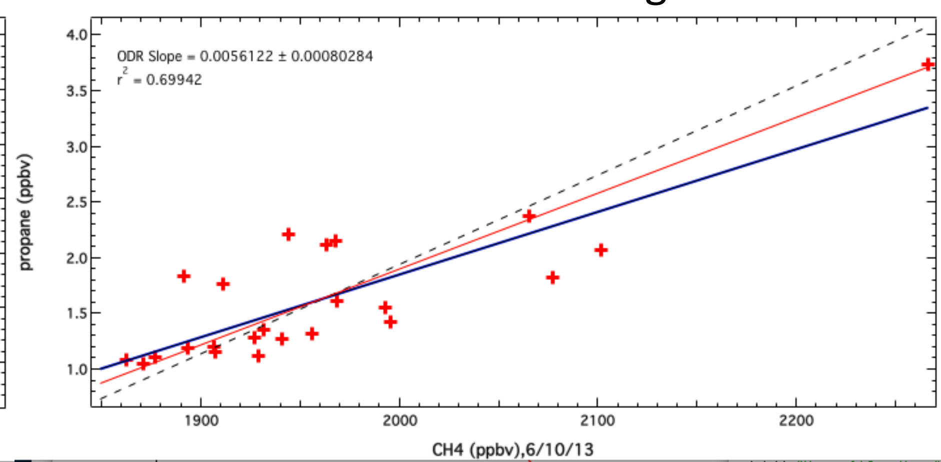
Haynesville, 6/10/13 flight



West of 93.75° W longitude



East of 93.75° W longitude



Oil and natural gas sector emissions for the Uinta Basin used in the model

Emission datasets	Source	Methane (tons/year)	Non methane VOCs (tons/year)	NO_x (tons/year)
Bottom-up	EPA National Emission Inventory (NEI-2011)	100,279	101,184	16,448
Top-down	Based on the measurements	482,130	184,511	4,158

Ahmadov et al. (2015), ACP

- ✓ Total top-down based methane flux estimate is from *Karion et al., 2013*
- ✓ Total methane and other VOC emissions in NEI-2011 are lower by a factor of 4.8 and 1.8 than in the top-down estimates respectively!
- ✓ Conversely, NO_x emissions are 4 times higher in the NEI-2011 inventory!

Implications for air quality regulations, climate and air quality studies!