Top-Down Estimation of Emissions from Oil and Gas Production and their Impact on Air Quality within a Regional Air Quality Model

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Field Studies with 15 to 50 VOC, CH_4, and Observed CH_4 Emissions

Uintah Basin Wintertime Ozone Study (2012,2013)

Karion et al., GRL, 2013
CH_4 flux = 1450 ton/day

R. Ahmadov, et al., ACP, 2015

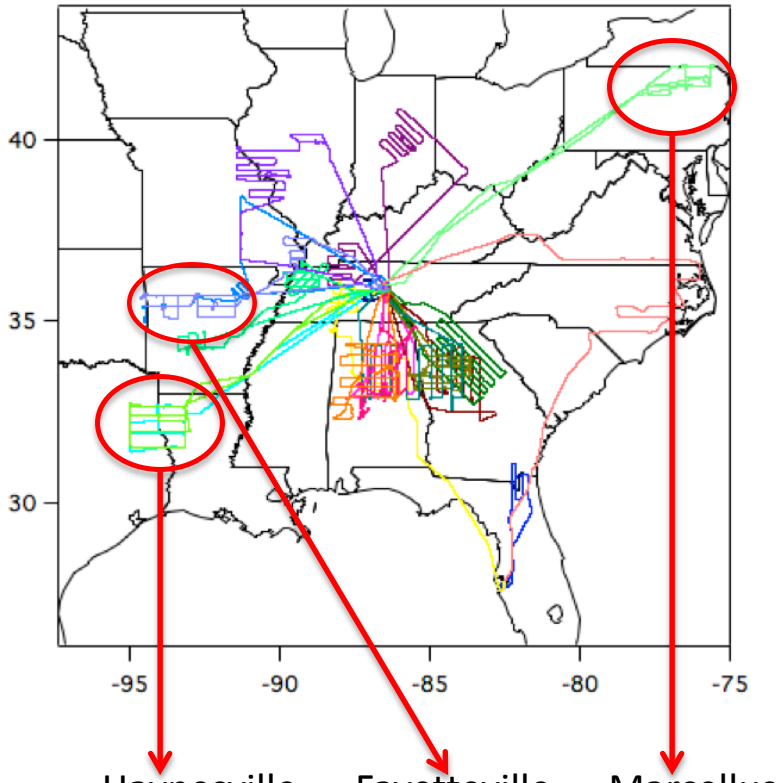
DJB

Summertime Ozone Near Natural Gas Emissions (SONNE)
July/August, 2012

G. Petrón et al., JGR, 2014
CH_4 flux = 510 ton/day

J. Gilman, et al., EST, 2013

Southeast Nexus (SENEX)
June/July 2013,southeast U.S.



CH_4 flux, ton/day

J. Peischl, et al., JGR, 2015

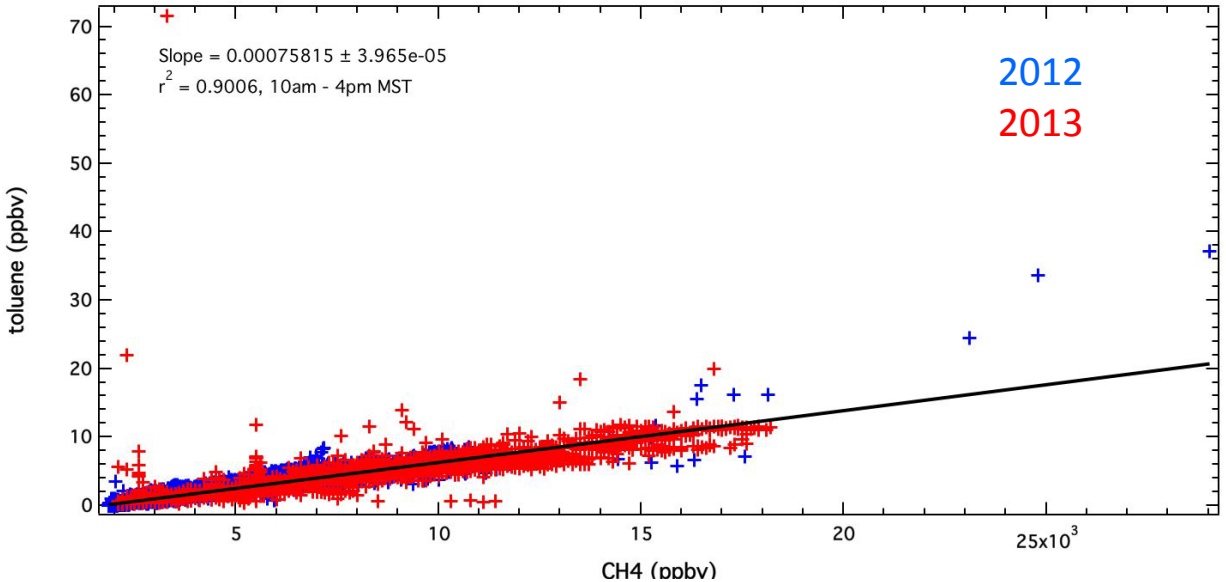
Background Example: Uintah Basin 2012/2013 Study (Ahmadov et al., 2015)

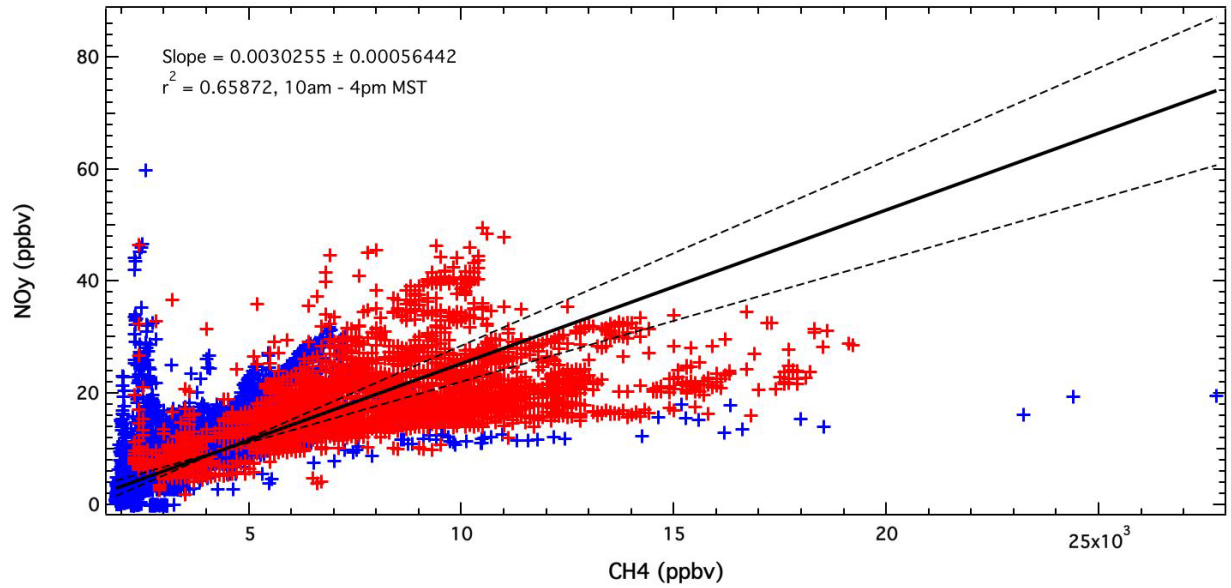
Oil and Gas Production Inventories used in emission comparison and model study

1) **Bottom-up:** NEI-2011 (version 1)
   Uses - V1 model platform metadata (available 11/8/13)
   SPECIATE 4.3 VOC speciation
   WRAP-III VOC and NOx emissions for 9 O&G Basins

2) **Top-down**: VOC/CH_4 and NOy/CH_4 ratios from Horse Pool observations during winters of 2012 and 2013
   Karion et al (2013) CH_4 fluxes determined from aircraft during winter of 2012

Examples of CH_4 regressions, VOC/NOy measurements at the Horse Pool site





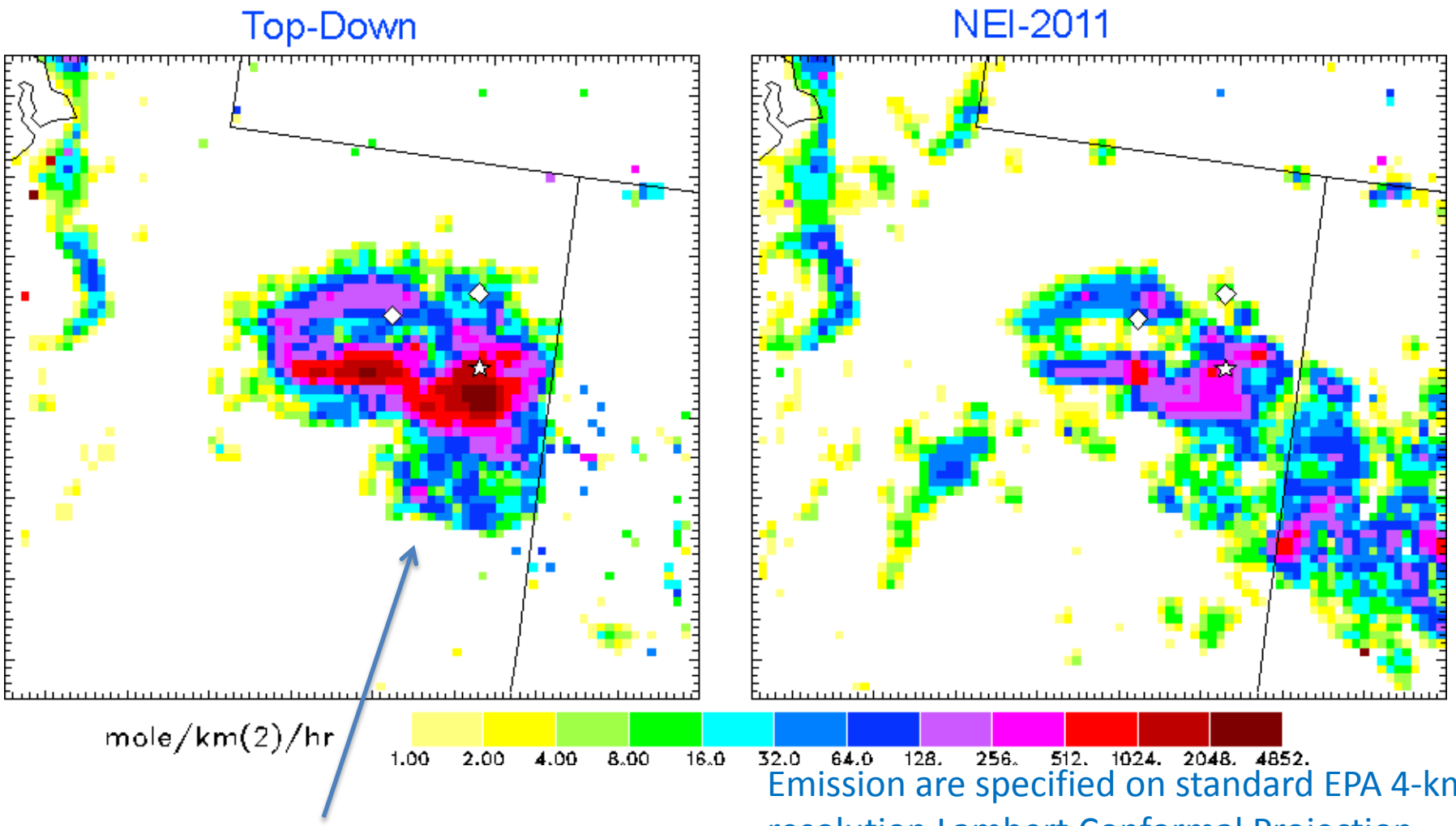
10:00 am to 4:00 pm LST

VOC from GC-MS
(J. Gilman, B. Lerner)
10 minute data

CH_4 from Picarro
(J. Peischl)
one minute data

NOy from
Chemiluminescence
(E. Williams)
one minute data

Diurnal average CH_4 fluxes from both inventories



Emission are specified on standard EPA 4-km resolution Lambert Conformal Projection

Oil and gas well locations are from the Utah Department of Oil, Gas and Minerals (May, 2012)

Oil and gas emission totals (Uintah and Duchesne Counties)

Inventory	Source Tons/Year	NO_x	VOC	CH_4
NEI-2011	Oil & Gas	18,131	111,536	110,539
	All Other Activity	4,514	3,047	1,597
	Bonanza Power Plant	6,590	46	-
NEI-2005	Oil & Gas	-	-	-
	All Other Activity	2,585	3,525	1,231
	Bonanza Power Plant	6,712	63	-
Top-down	Oil & Gas	4,583	203,389	531,457

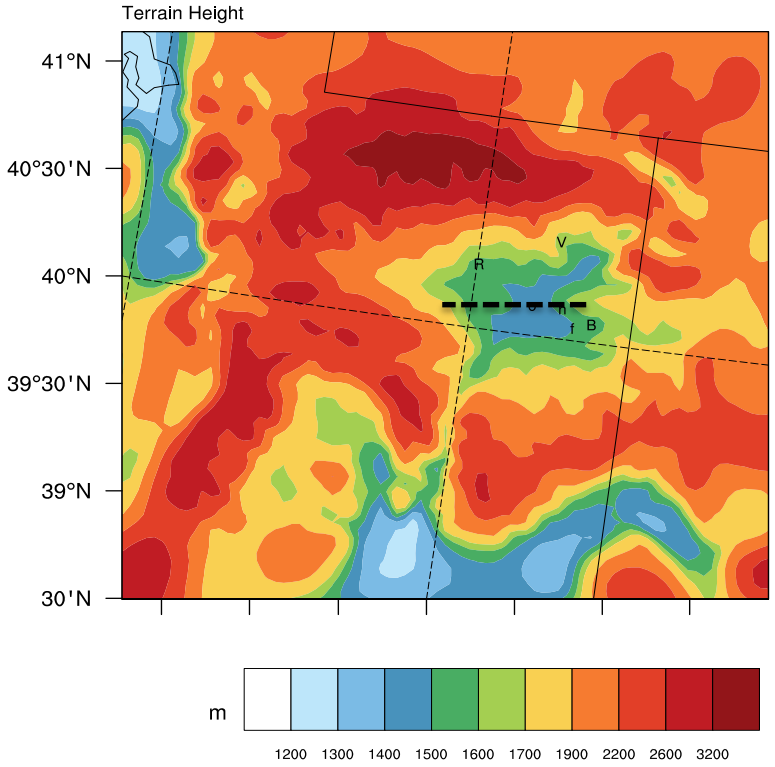
Total CH_4 flux for Top-down is from *Karion et al., 2013*

Total CH_4 and NMVOC emissions in NEI2011 are lower by a factor of 4.4 and 1.6 than in the top-down estimates respectively.

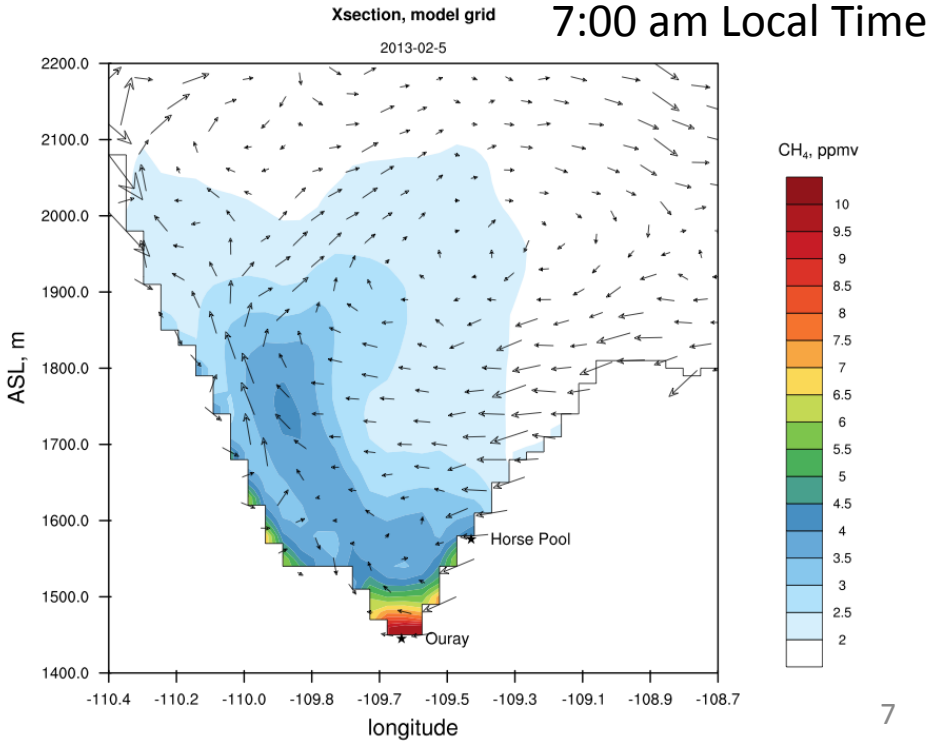
Conversely NOx emissions are 4. times higher in the NEI2011 inventory.

WRF/Chem Model, Uintah Basin Studies of 2012, 2013
Ahmadov et al., ACP, 2015

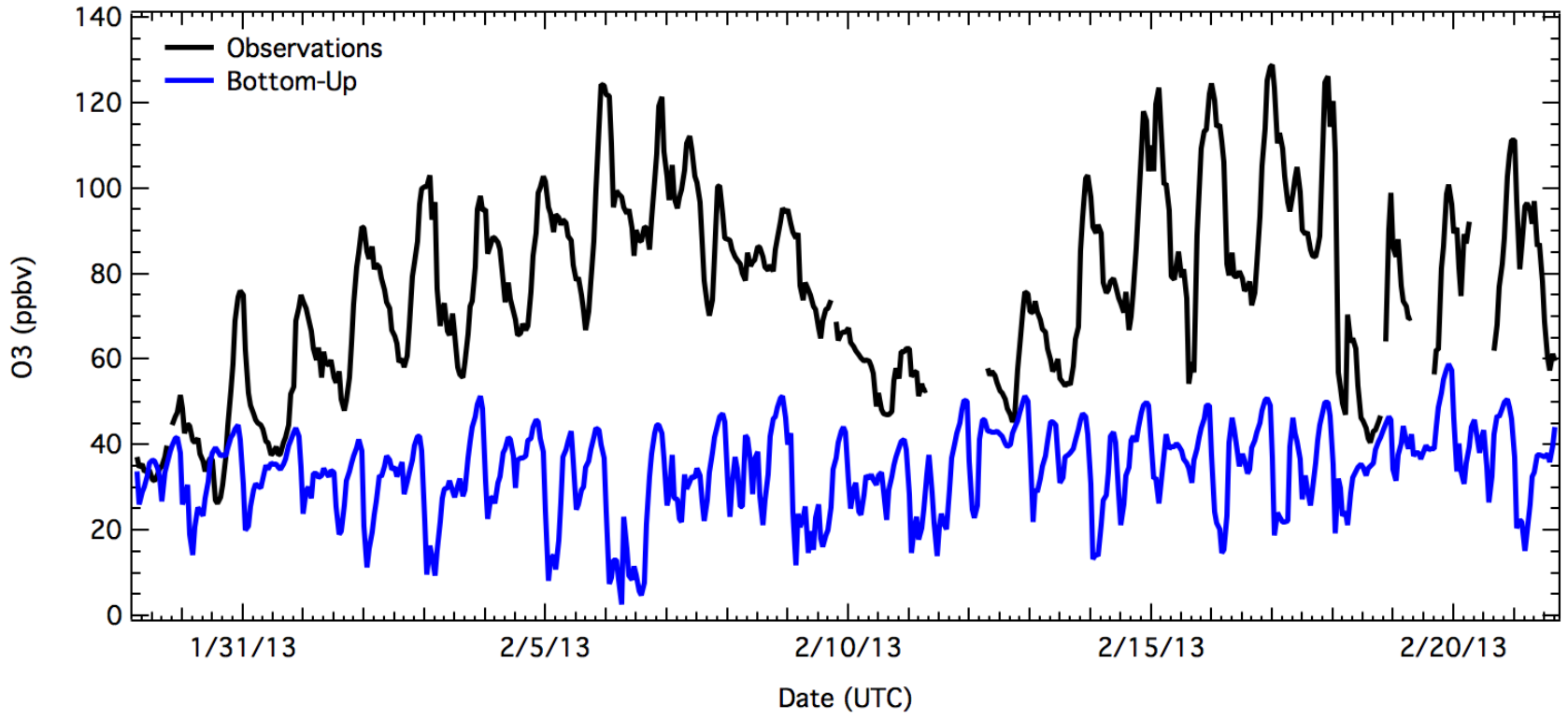
Horizontal resolution	12 and 4 km nested domains
Vertical resolution	60 layers (18 within lowest 500m)
Meteorological input	NAM analysis
PBL and surface layer schemes	Mellor-Yamada Nakanishi and Niino
Land Surface	Noah Land Surface Model
Microphysics	WRF Single-Moment 5-class
Shortwave and longwave radiation	RRTMG
Gas-phase chemistry	RACM_ESRL
Transport of species	advection and vertical mixing
Advection option for chemical variables	Monotonic



CH4 mixing ratio
7:00 am Local Time

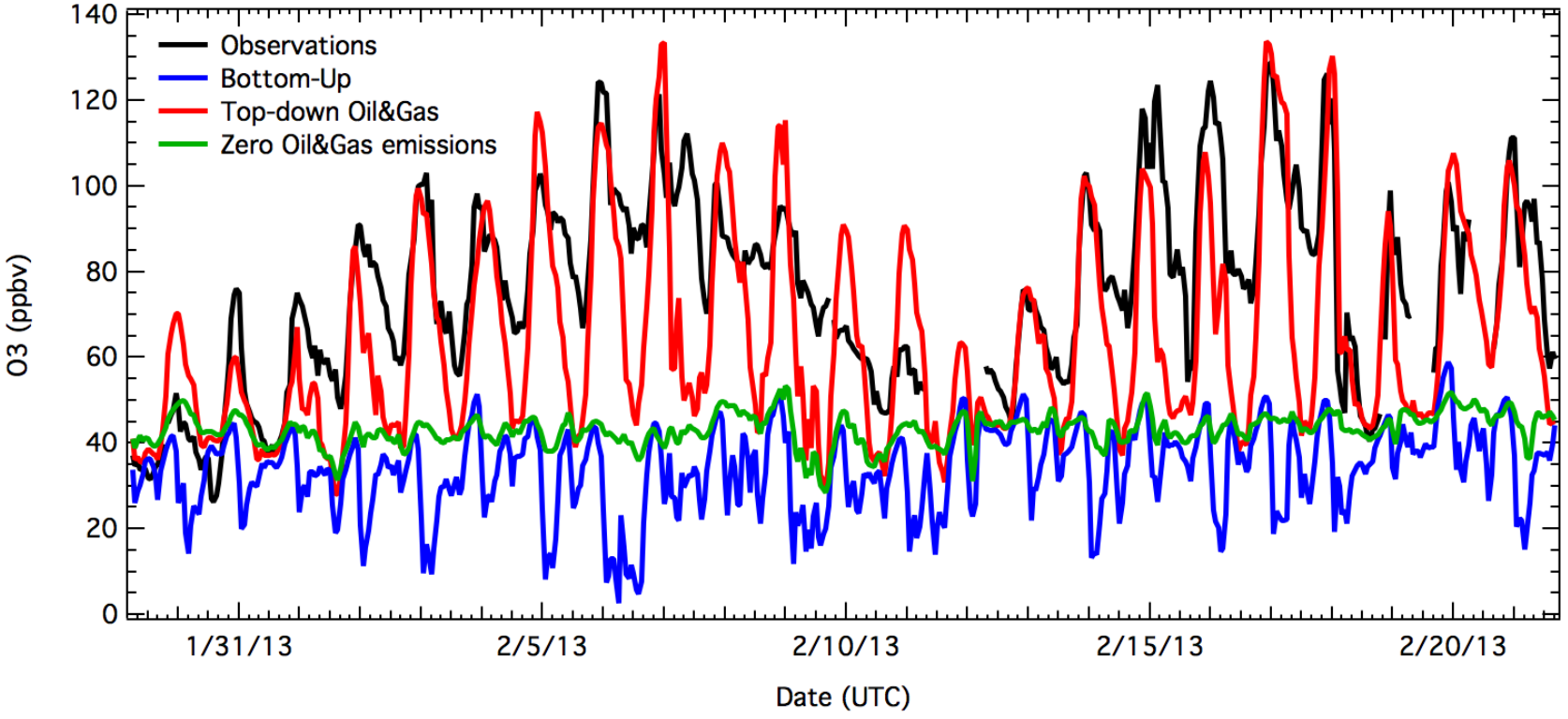


Observed and modeled ozone time series at the Horsepool site



Observed and modeled ozone time series at the Horsepool site, 2013

Daytime (9-17MST) statistics:
Bottom-up case: *r= 0.33, med. bias= -39.8 ppb, med. (mod./obs.)= 0.51*
Top-down case: *r= 0.85, med. bias= -5.3 ppb, med. (mod./obs.)= 0.93*



Oil/Gas Sector Emissions used in the 5-Basin model comparisons (Model runs for summertime June/July SENEX-2013 period)

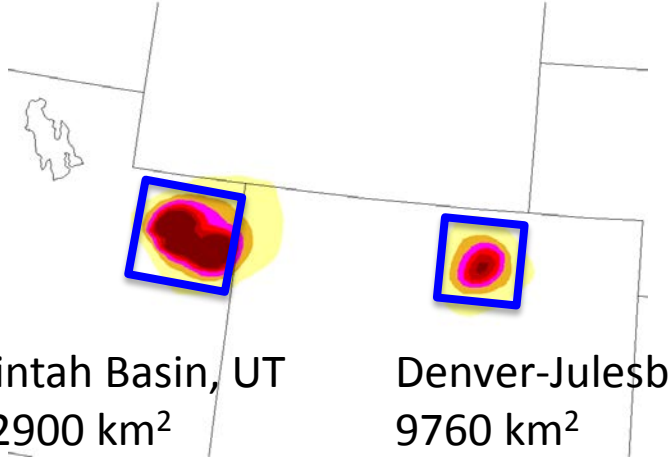
1) **Base – No Oil/Gas activity emissions:**
   NEI-2011 (version 1) with Oil/Gas sources removed over entire U.S.
   Nonpoint SCCs: 2310000000-2310199999 removed
   Point: 31000101-31088811, 40400300-40400340, 30600801-30600999

2) **Bottom-up:** Base emission case with NEI-2011 in 5 Basins:
   Version 2 Oil/Gas sector SCC to VOC profile assignments.
   (gsref_voc_2011v2_platform_05jan2015_v5.txt)
   SPECIATE 4.4 VOC speciation for oil/gas sector.

3) **Top-down**: Base emission case with Top-Down data in 5 Basins:
   VOC and NOy correlations with CH_4 from each basin.
   CH4 emissions from aircraft measurements (mass-balance technique)
   Spatial allocation normalized according to NEI-2011, version 1 VOC.

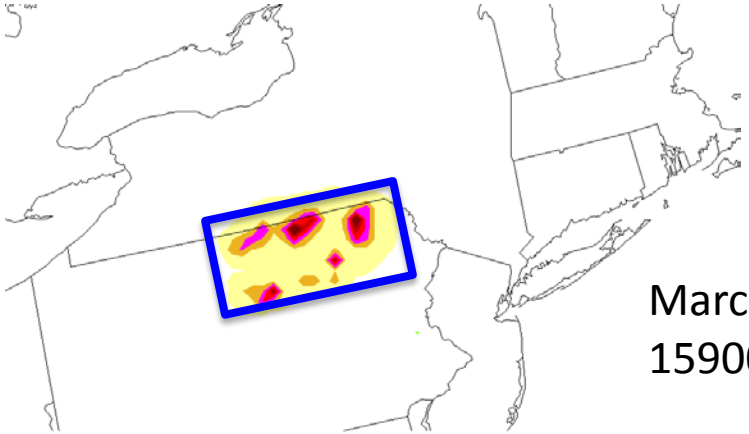
Latitude and Longitude Limits of the 5 Basins

Emission Boxes determined from Aircraft Sampling Limits
(Karion et al., 2013; Petrón et al., 2014, Peischl et al., 2015)



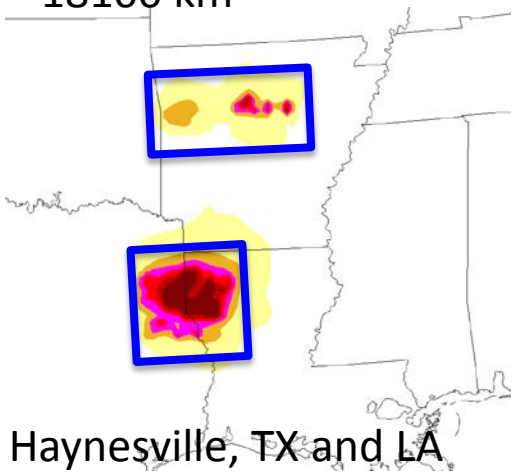
Uintah Basin, UT
12900 km^2

Denver-Julesburg, CO
9760 km^2



Marcellus, PA
15900 km^2

Fayetteville, AR
18100 km^2



Haynesville, TX and LA
23250 km^2

Top-Down NOy and VOC to CH_4 emission ratios for the 5 Basins

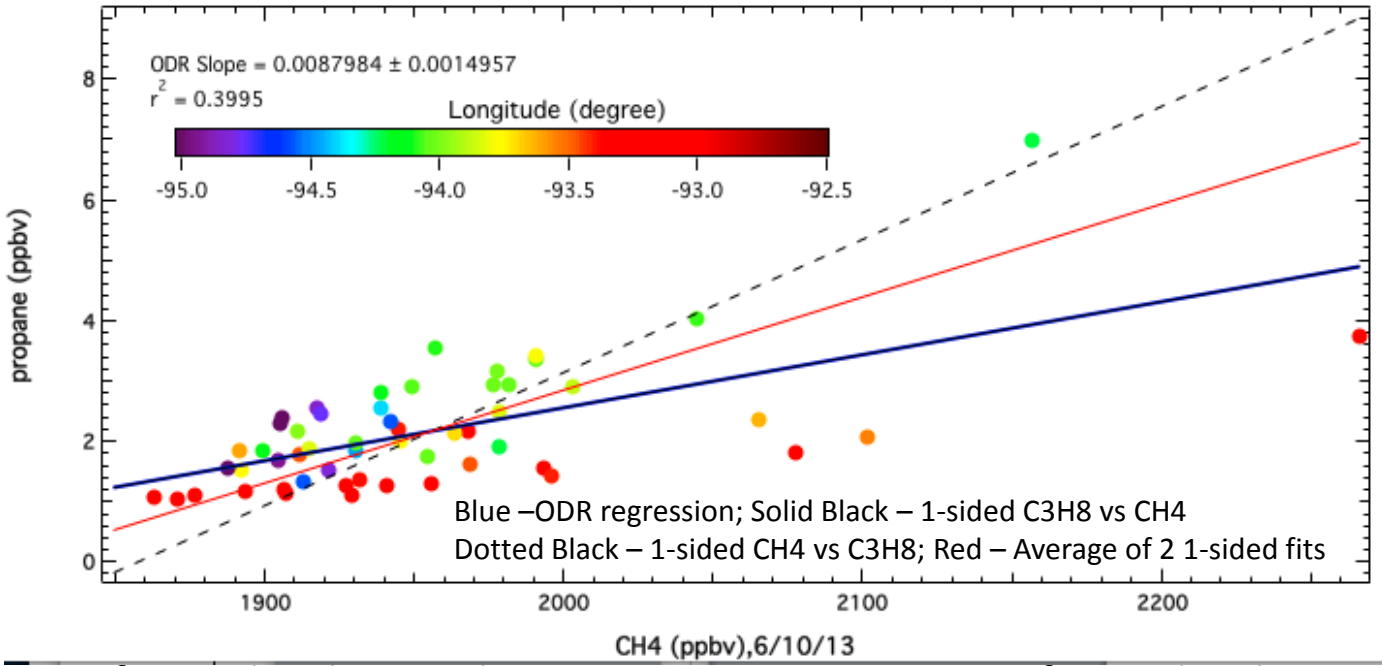
Uintah Basin: From Ahmadov et al. (2015) – Winter O_3 studies

Denver-Julesburg: From SONNE (2012) Erie Tower Measurements
2-variable regression fits (propane, acetylene); Gilman et al. (2013)
NOx/CH4 oil/gas ratio = 0. for DJB
VOC/CH4 ratios agree with Petrón et al. (2014) (for 5 reported VOC)

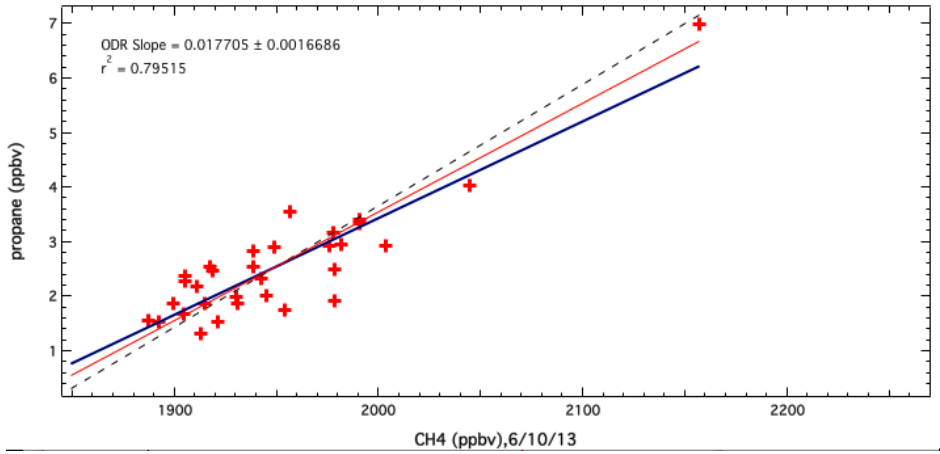
SENEX-2013 aircraft: Orthogonal linear regressions – no weighting
VOC with significant CH_4 correlations ($r^2 > 0.5$) use calculated regressions as is.
VOC with lower CH_4 correlations use Uintah and DJB regressions, scaled to the lightweight alkane having equivalent difference between Uintah and DJB ratios (relative to CH_4).

Example of SENEX-2013 regressions: C_3H_8 versus CH_4

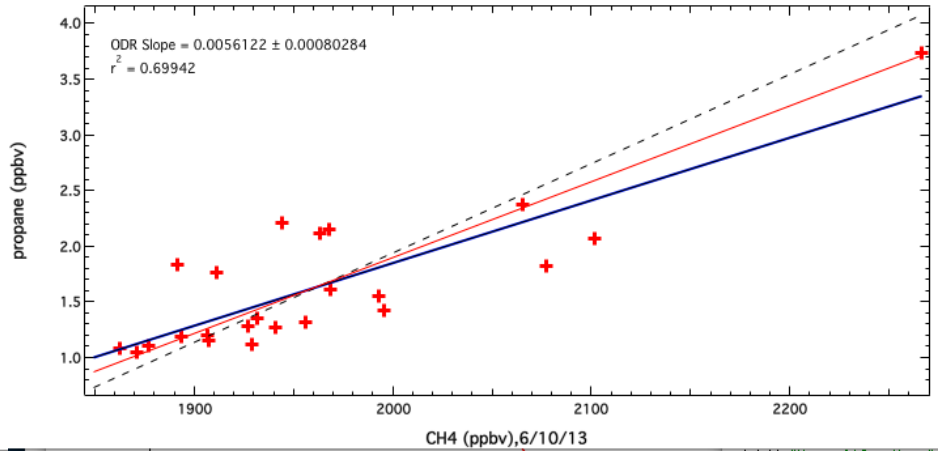
Haynesville, 6/10/13 flight



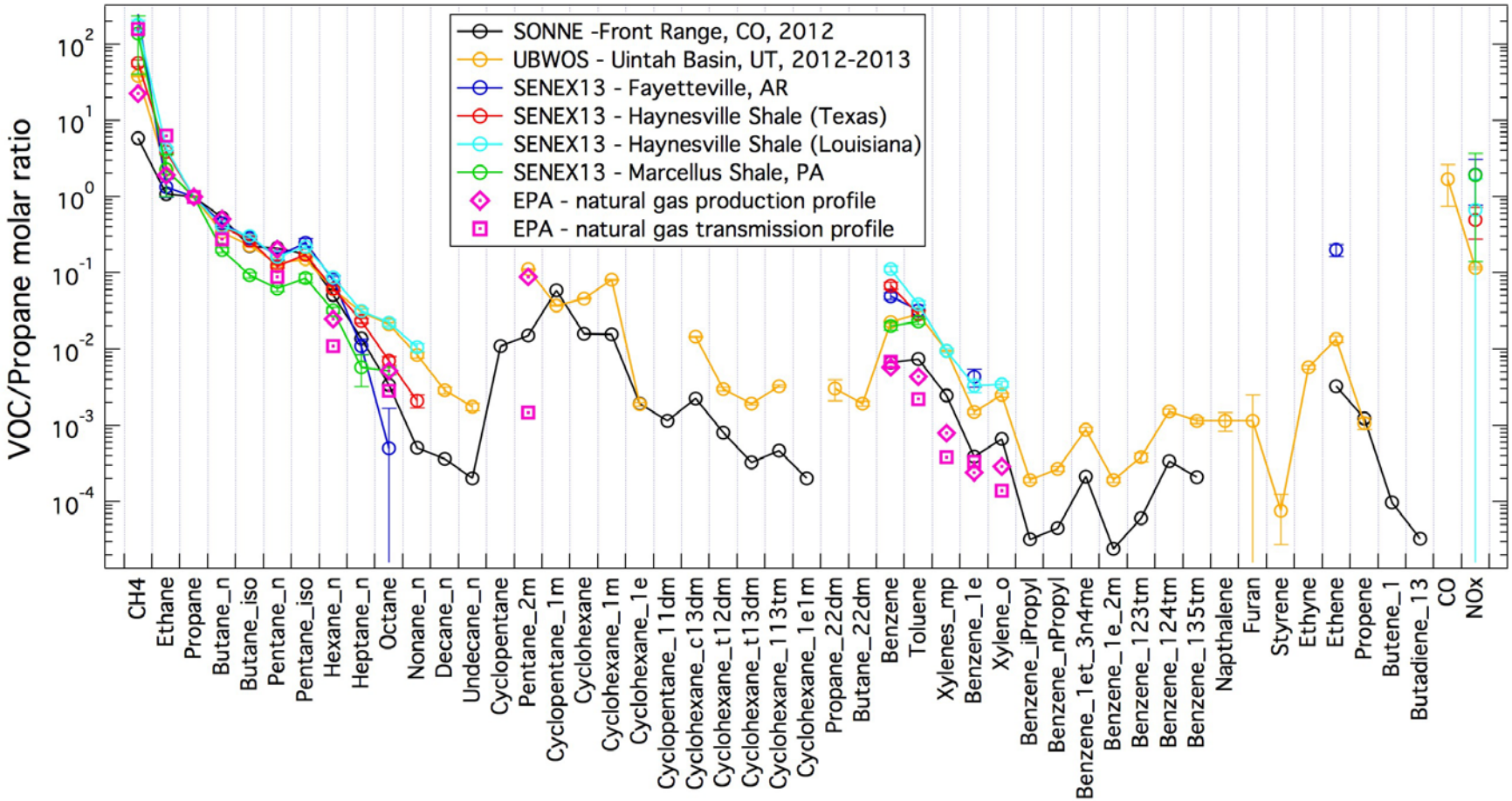
West of 93.75° W longitude



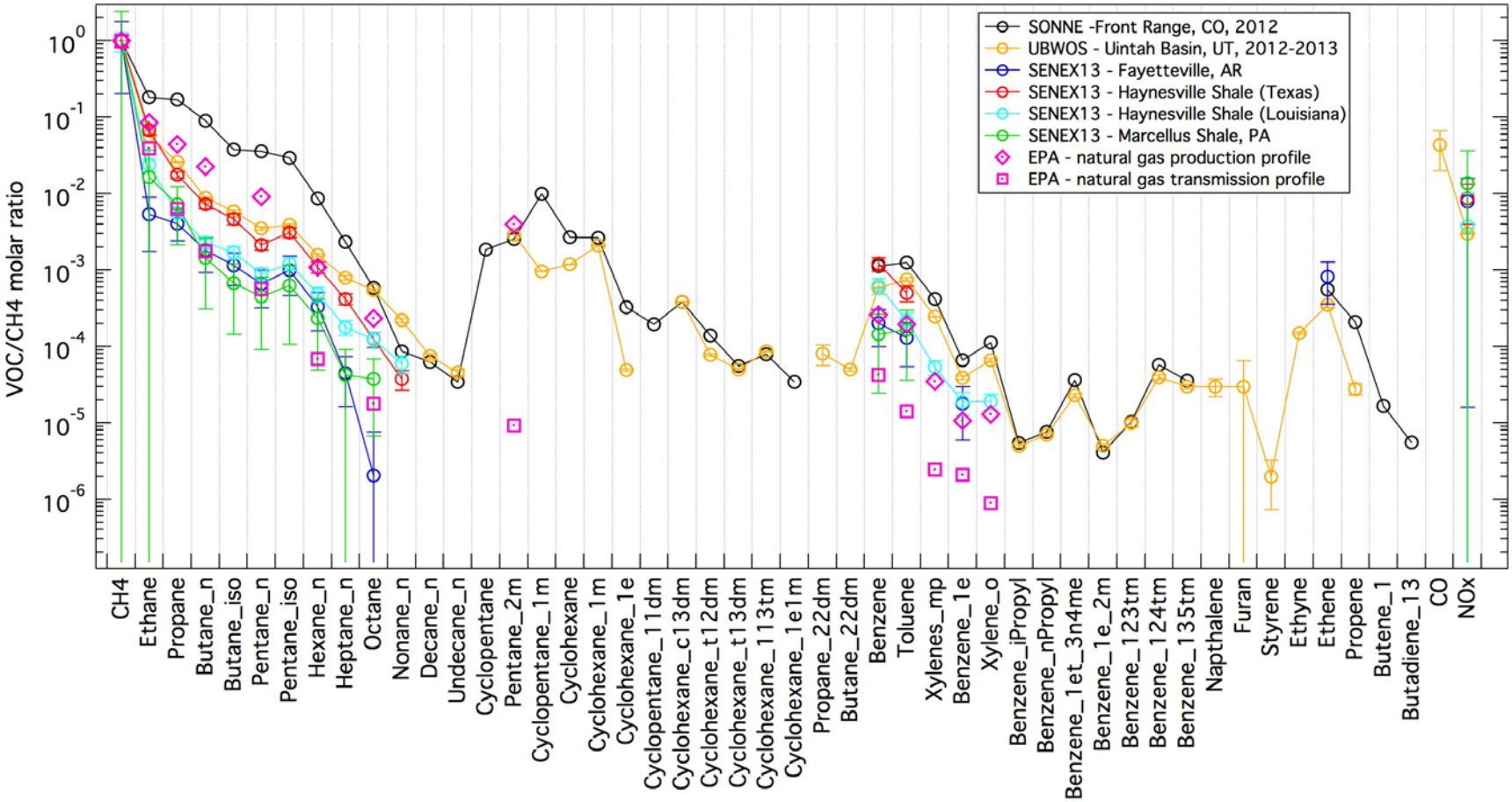
East of 93.75° W longitude



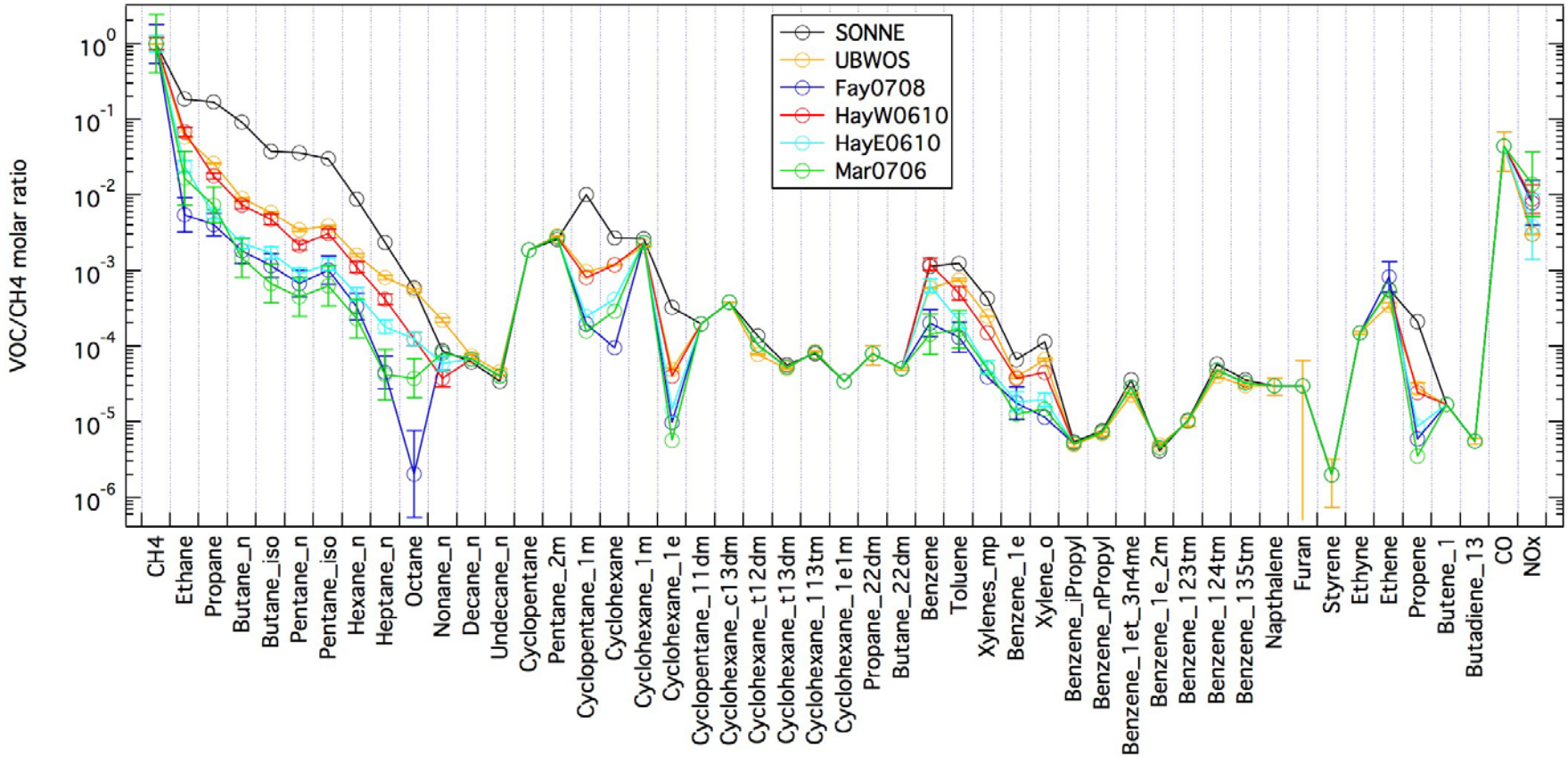
Top-Down VOC and NOx regression slopes – relative to Propane



Top-Down VOC and NOx regression slopes – relative to CH_4



Adopted VOC and NOx emission ratios – relative to CH_4



NOx emissions Top-Down versus NEI-2011 for all 5 Basins

NOx emissions (ton/day) in the 5 Basins

Basin	Top-Down O&G	NEI-2011v2 O&G		NEI-2011 on and off road	NEI-2011 point
Uintah	12.6	53.6		8.3	24.3
Denver-Julesburg	0.0	18.4		90.5	68.2
Haynesville/West	17.5	56.1		50.6	86.1
Haynesville/East	15.5	41.1		55.7	35.0
Fayetteville/West	19.8	13.2		37.9	5.0
Fayetteville/East	23.4	15.4		16.4	11.3
Marcellus	15.7	23.5		61.7	6.4

Top-Down Oil/Gas sector NOx emissions are much lower than NEI-2011, except for the Fayetteville Basin.

NOx emission differences are significant, relative to mobile onroad/nonroad sources, except for the Denver-Julesburg Basin.

The Top-Down Oil/Gas sector NOx emissions are upper limits, since part of the NOx/CH4 observed correlation may have onroad/nonroad contributions.

VOC emissions Top-Down versus NEI-2011 for all 5 Basins

Toluene emissions (kmole/day)

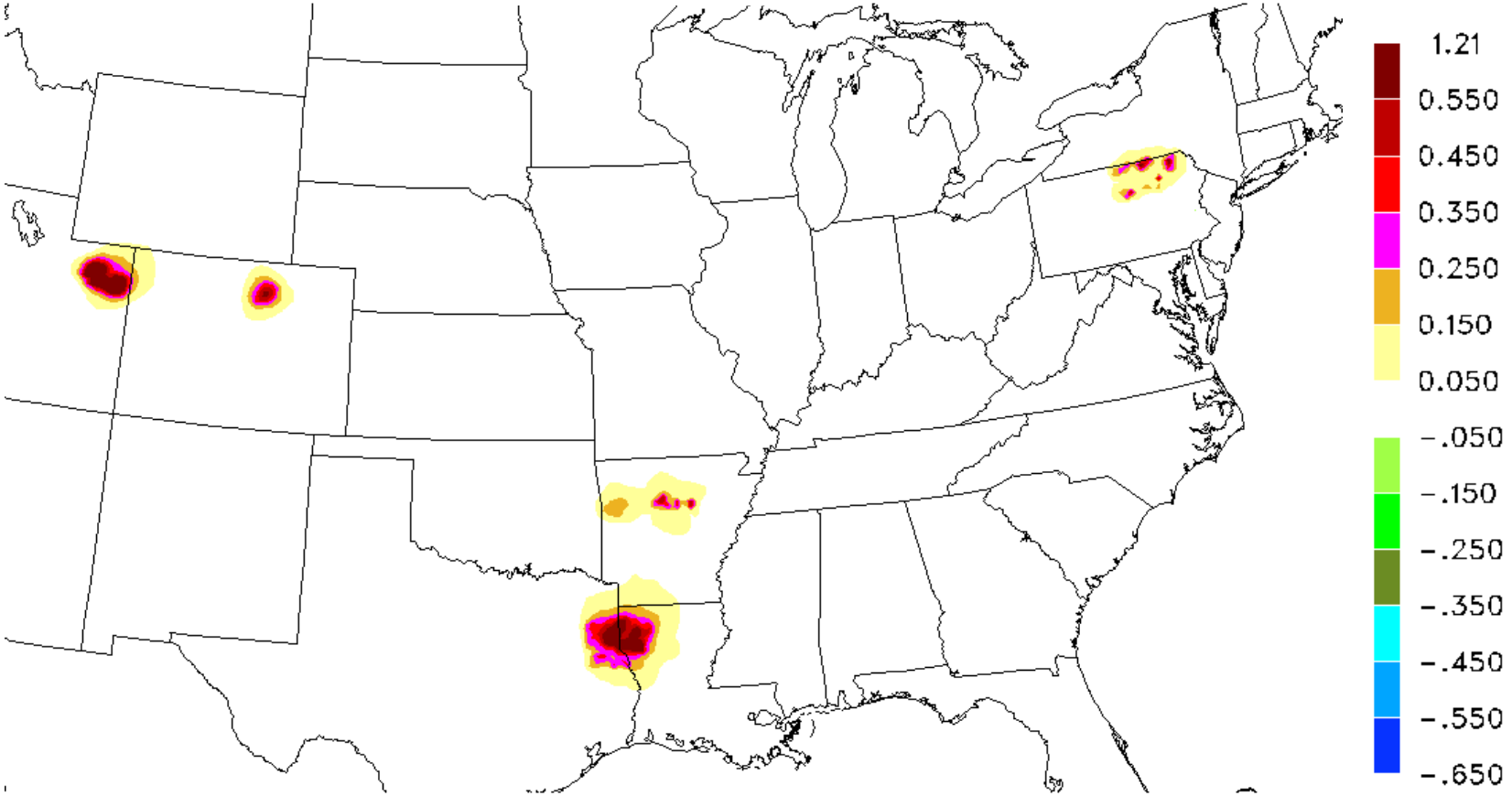
Basin	Top-Down O&G	NEI-2011v2 O&G		NEI-2011 on and off road	NEI-2011 point
Uintah	62.7	15.9		4.2	6.0
Denver-Julesburg	36.5	9.5		60.6	12.4
Haynesville/West	19.9	5.1		20.7	4.8
Haynesville/East	17.4	2.0		35.2	10.2
Fayetteville/West	6.5	0.3		14.8	1.2
Fayetteville/East	7.7	0.4		13.9	0.8
Marcellus	3.8	0.06		45.7	1.7

Top-Down Oil/Gas sector VOC emissions are much higher than NEI-2011.

Top-Down Oil/Gas sector VOC dominate or comparable to anthropogenic VOC sources, except in the Marcellus Basin.

June 2013 average, 19:00 UTC

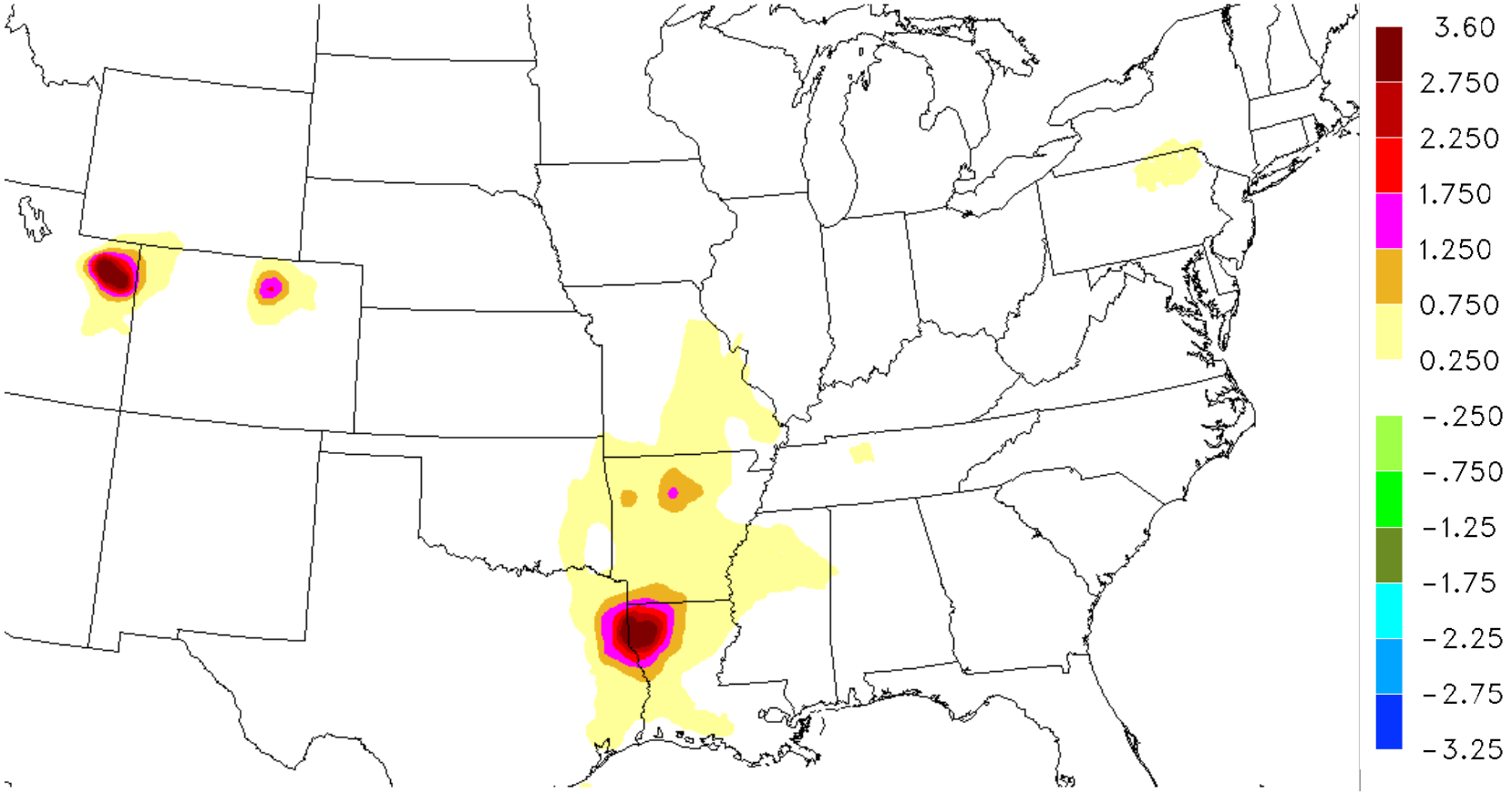
NEI-2011 NOy diff (ppbv)



Control = NEI-2011 version 1, Oil/Gas activity emissions removed
Perturbation = Control with NEI2011 version 2 O/G activity emissions included

June 2013 average, 19:00 UTC

NEI-2011 O_3 diff (ppbv)

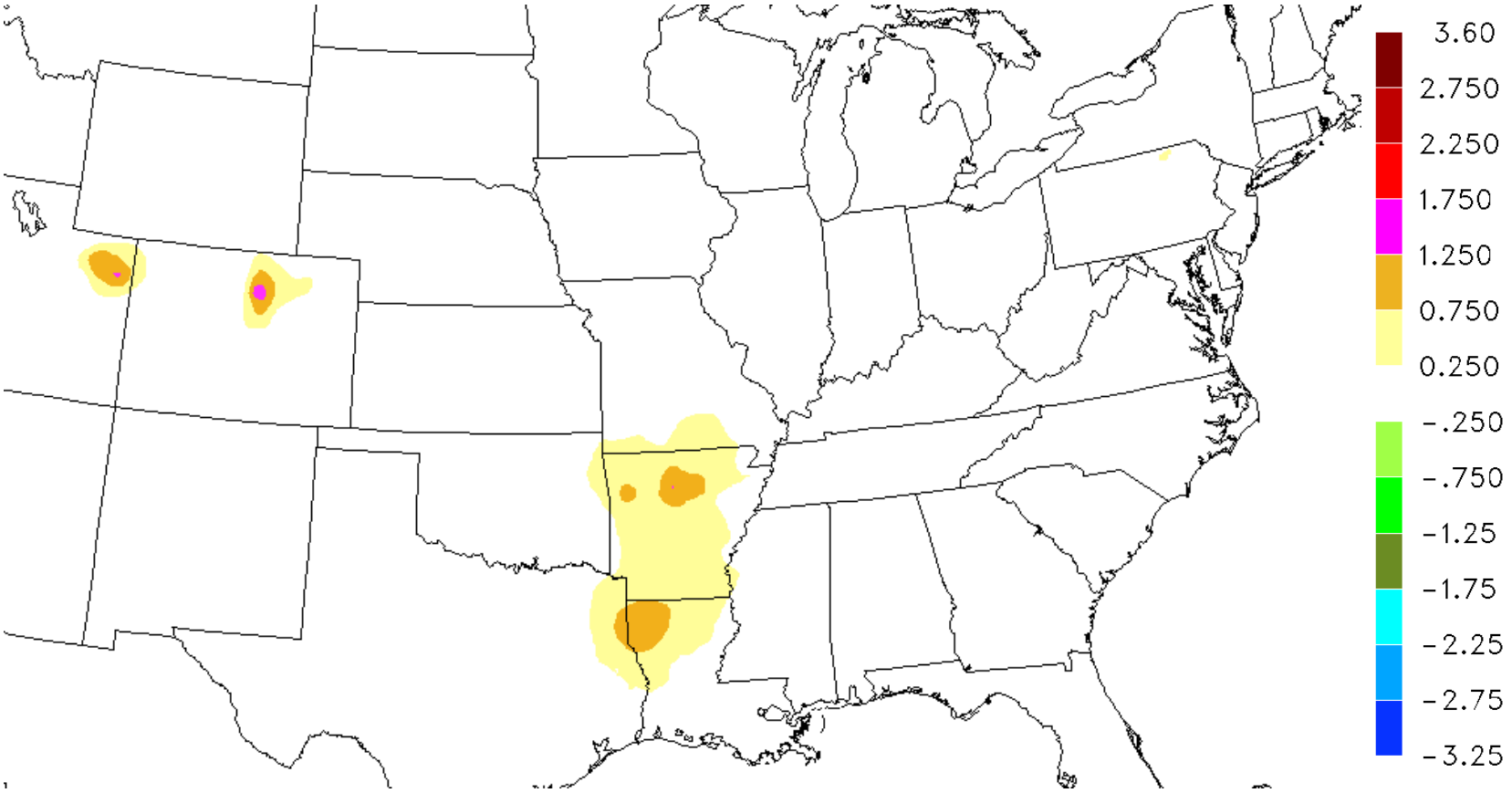


Control = NEI-2011 version 1, Oil/Gas activity emissions removed

Perturbation = Control with NEI2011 version 2 O/G activity emissions included

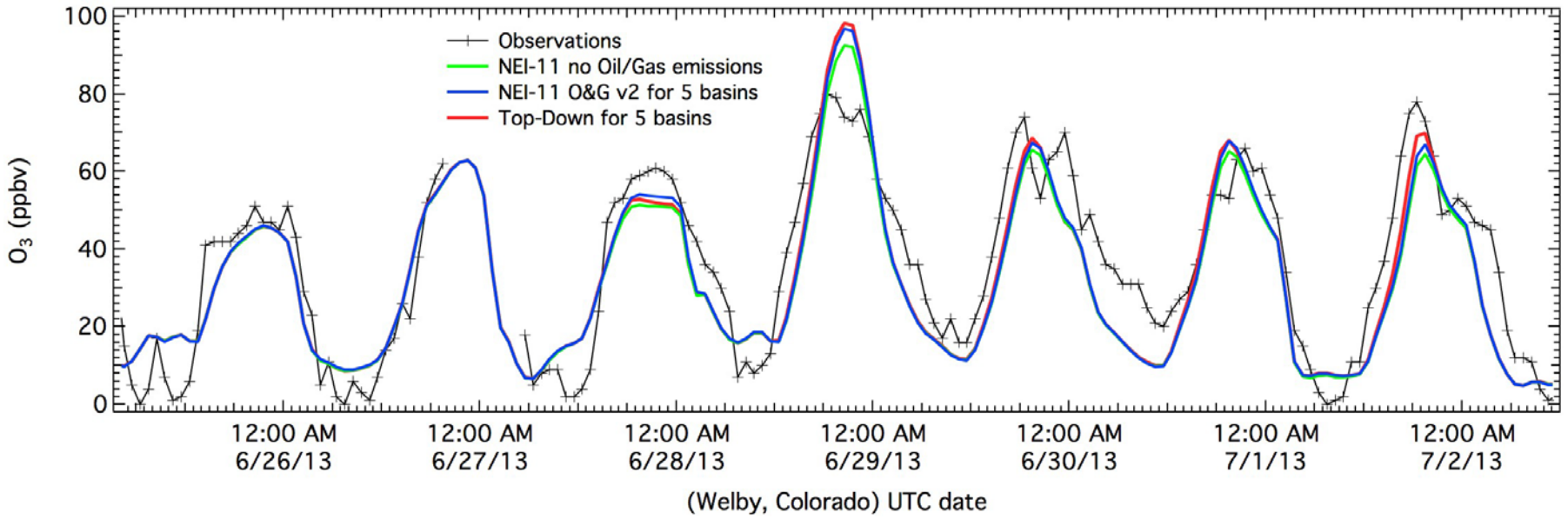
June 2013 average, 19:00 UTC

Top-Down O_3 diff (ppbv)



Control = NEI-2011 version 1, Oil/Gas activity emissions removed
Perturbation = Control with Top-Down Emissions for 5 basins

Model predicted maximum O_3 differences (June/July 2013) (coincident with O_3 monitor location)



Top-Down Emissions:

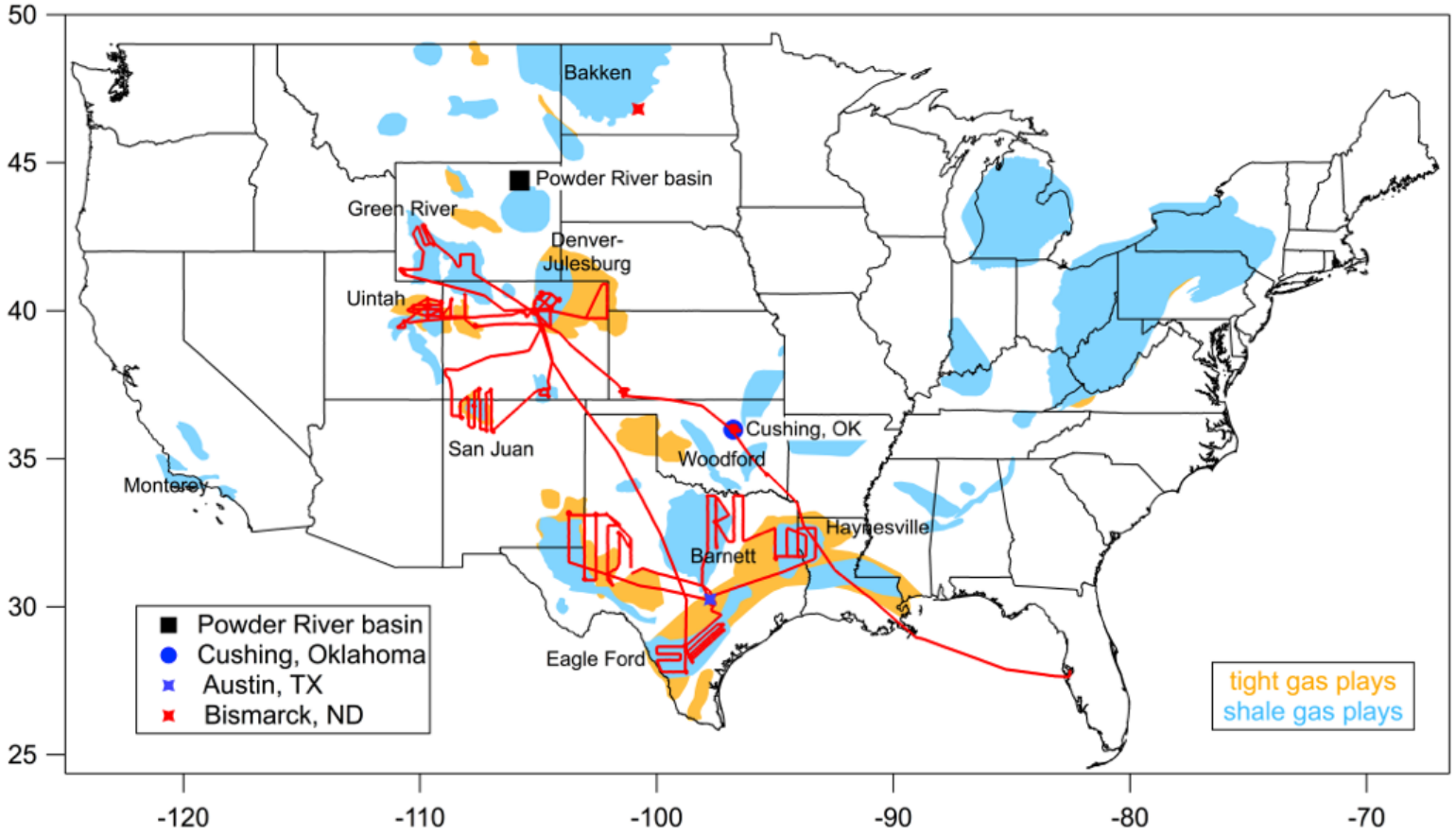
Maximum Oil/Gas Impact on O_3 = 8.5 ppbv, Northeast of Denver
(8-hr average O_3 difference = 3.8 ppbv)

NEI-2011, version 2 Oil/Gas:

Maximum Oil/Gas Impact on O_3 = 11.4 ppbv, Uintah Basin
(8-hr average O_3 difference = 4.9 ppbv)

Shale Oil and Natural Gas Nexus (SONGNEX-2015)
March 22 – May 1, 2015

Flights Completed as of April 6, 2015



Summary

- CH_4 emissions, NOy and VOC/CH_4 ratios from oil/gas activity in 5 Basins were used to derive Top-Down emission estimates of NOx and dozens of VOC species.

- Top-Down NOx emissions from the oil/gas sector are much lower than those from NEI-2011 for 4 out of 5 of the Basins.

- Top-Down VOC emissions from the oil/gas sector are much higher than those from NEI-2011.

- Oil/gas sector VOC speciation profiles from the new version 2 platform data are reasonably consistent with Top-Down estimates for < C7 normal alkanes. Aromatic emissions are too low (factor of 4-10) relative to CH_4 or C_3H_8, in all but one Basin.

- WRF/Chem model results show reduced impact from oil/gas activity emissions using the Top-Down inventory, compared to using NEI-2011 (version 2), due to reduced NOx emissions.

Additional Considerations

- The 5-Basin oil/gas inventory for CH_4, NOx, and 21 VOC is available for use on a 4-km EPA CONUS grid, zipped text files.

- Results from SONGNEX-2015 will be added, extending the Top-Down inventory to ~9 more basins.

- EPA guidance on spatial allocation within Basins?

- NOAA/CSD actively involved in inverse modeling of DJB and SENEX-13 sample regions.