Insight into Air Quality from Recent Measurement Campaigns and Model Runs

These are not unpleasant subjects; they are not uninteresting subjects; they are even exciting subjects – until one of these massive scientists gets hold of them. He soon convinces you that even these matters can be handled in such a way as to make a person low-spirited.

Mark Twain “A Tramp Abroad” 1880.

Supported by MDE
NIST, NASA, NOAA, and DNR
November 5, 2015

UMD/URF Cessna
Photo by J. Stehr

NASA & Air Quality

NASA Goddard Space Flight Center

Outline

- The ozone problem will not go away – new 70 ppb standard means both *larger* area of influence and need for *finer* resolution.
- Success story!
  - VOC controls help but,
  - Cities can't do it alone.
  - Regional NOx controls reduced regional O_3.
- What have we learned from science?

Air & Waste Management Association

em

THE MAGAZINE FOR ENVIRONMENTAL MANAGERS

FEBRUARY 2014

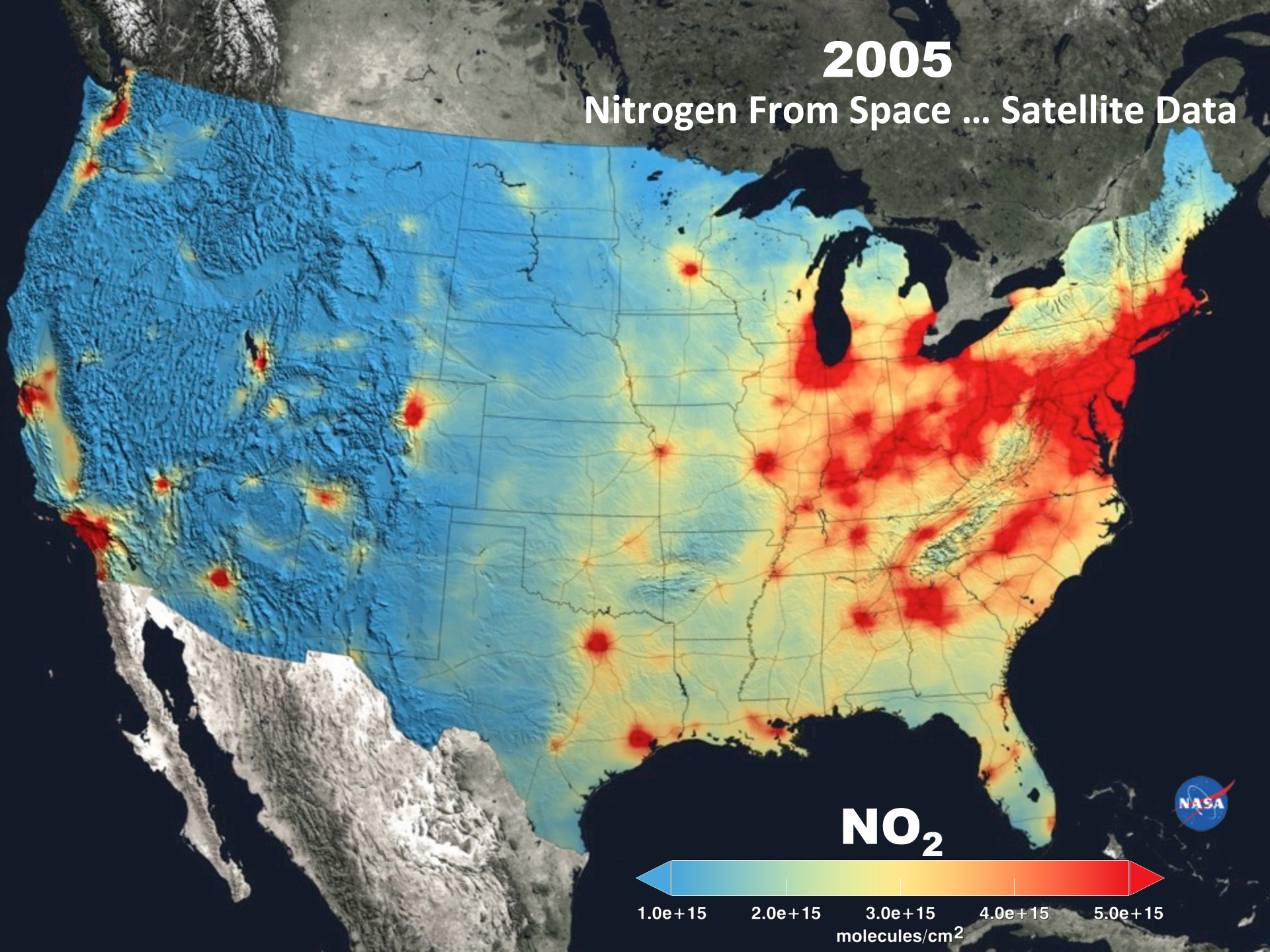
Also in this issue:

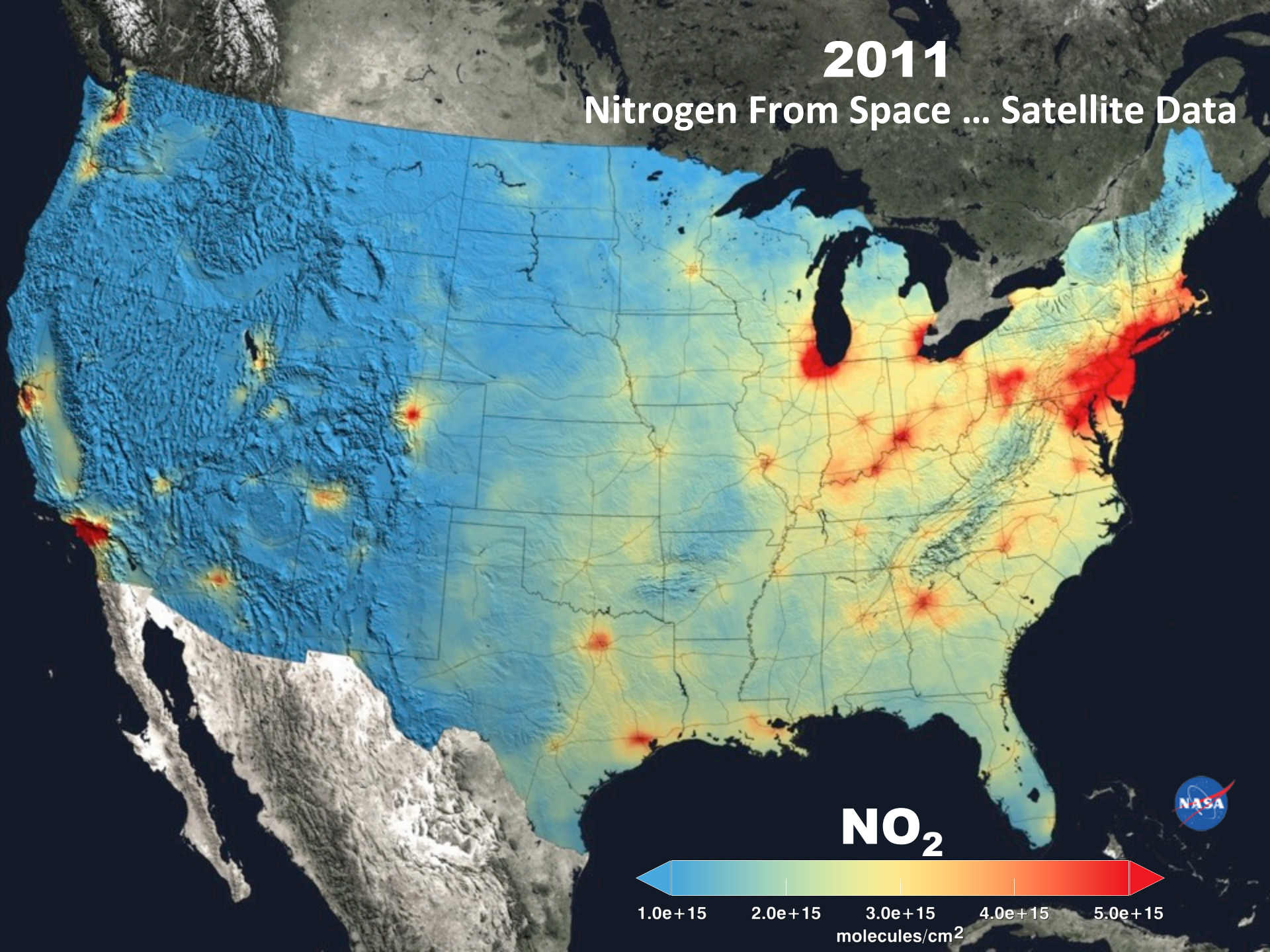
IT Insight: Can Windows and Other OSs Play in the Same Sandbox?

Asian Connections: Notes from the 1st Clean Fuels and Vehicles Forum in the ASEAN Region

Applying Satellite Data to Air Quality Management

Research conducted by the NASA Air Quality Applied Sciences Team (AQAST) shows that Earth science data are a great potential resource for air quality managers


2005
Nitrogen From Space … Satellite Data
NO2
1.0e+15
2.0e+15
3.0e+15
4.0e+15
5.0e+15
molecules/cm2
NASA


2011
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2.0e+15
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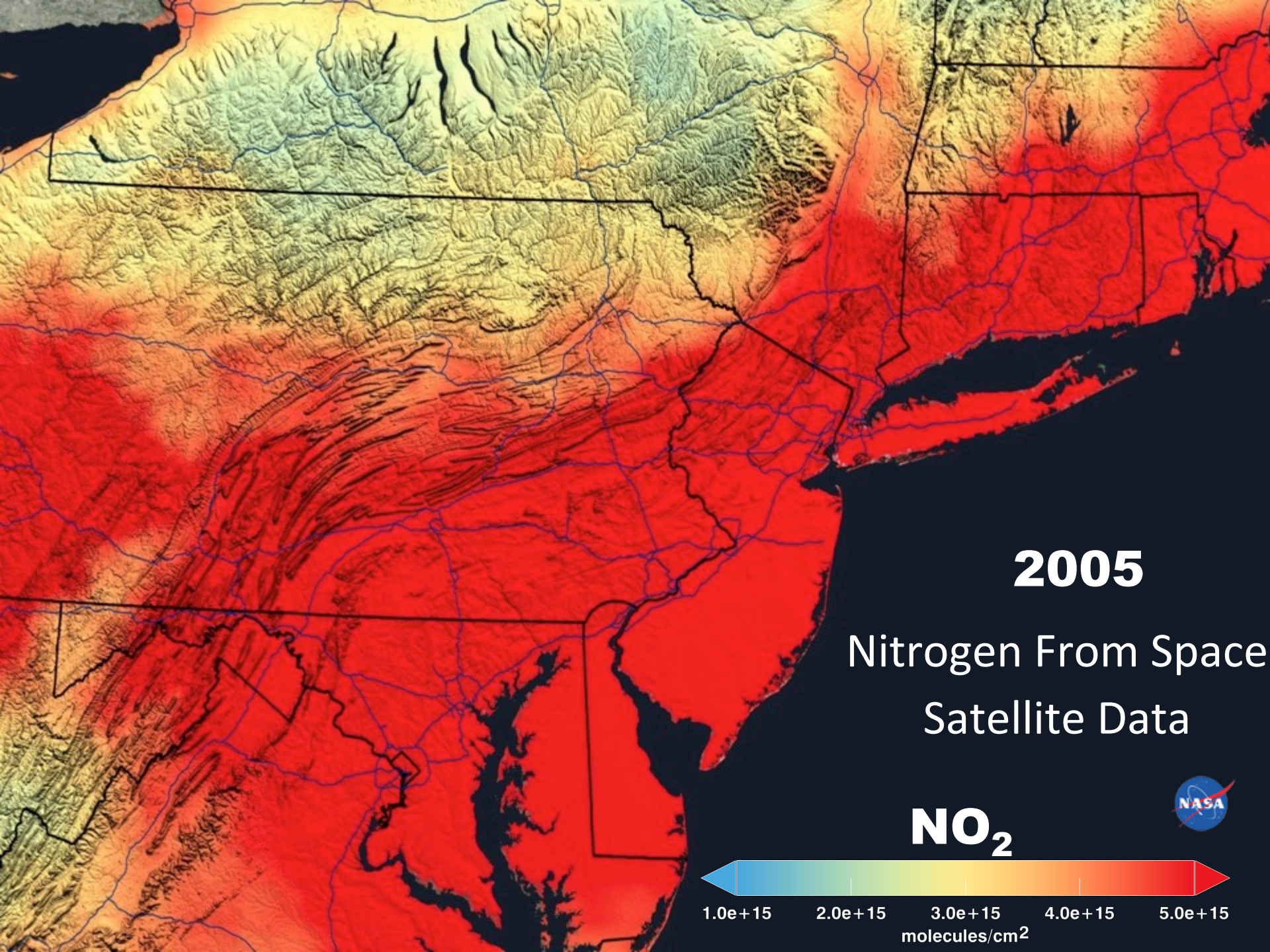
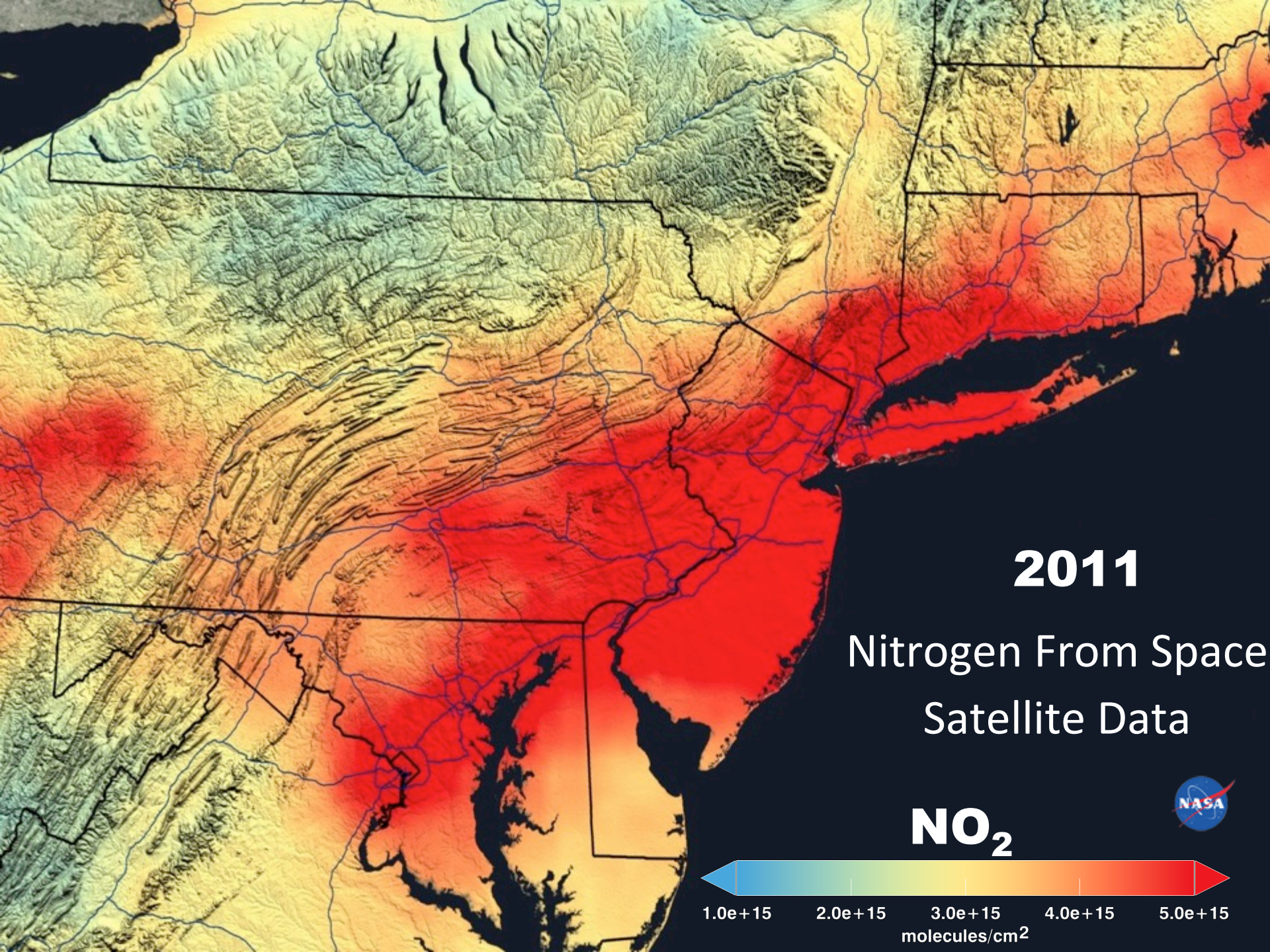
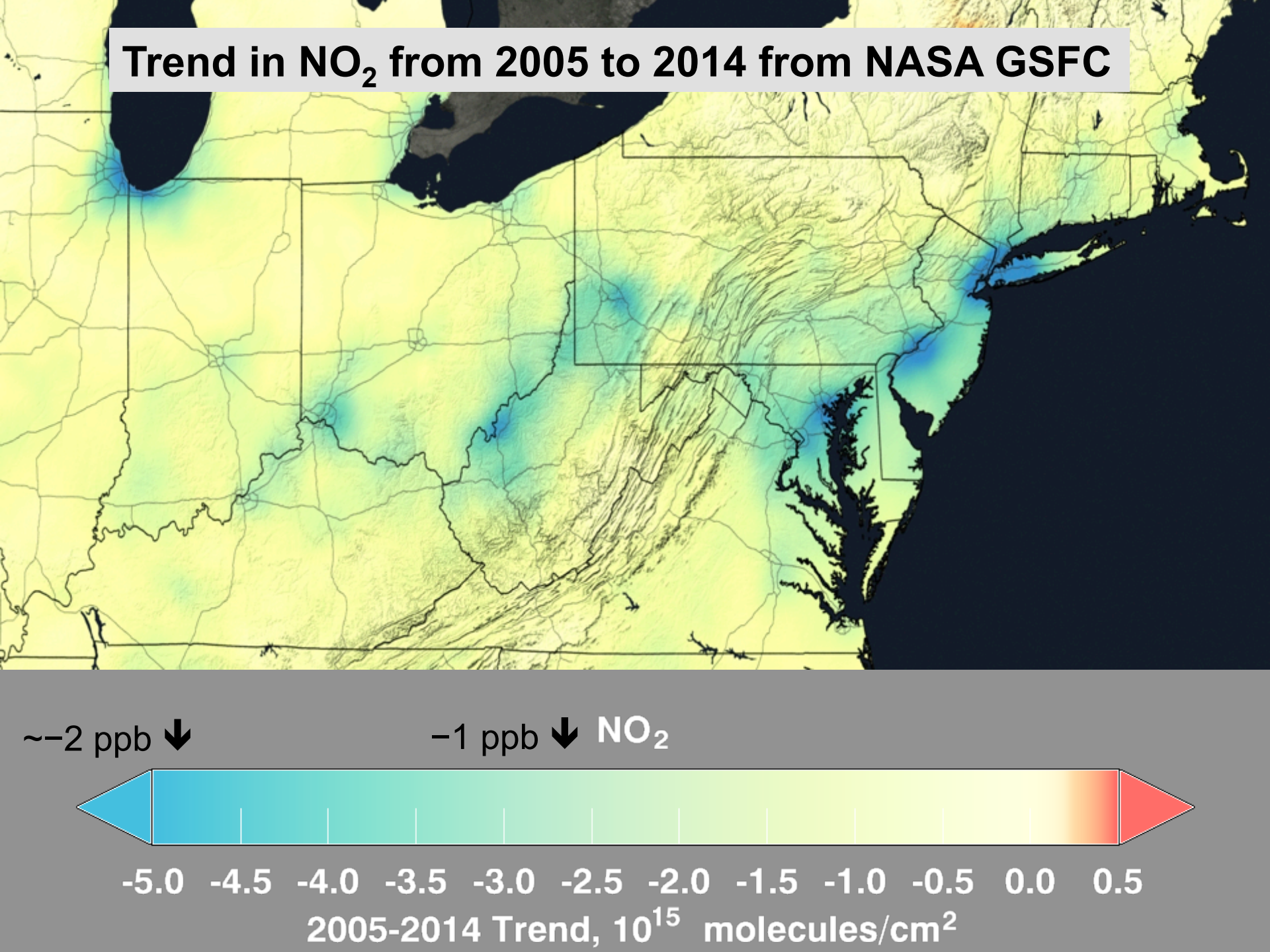
5.0e+15
molecules/cm2
NASA

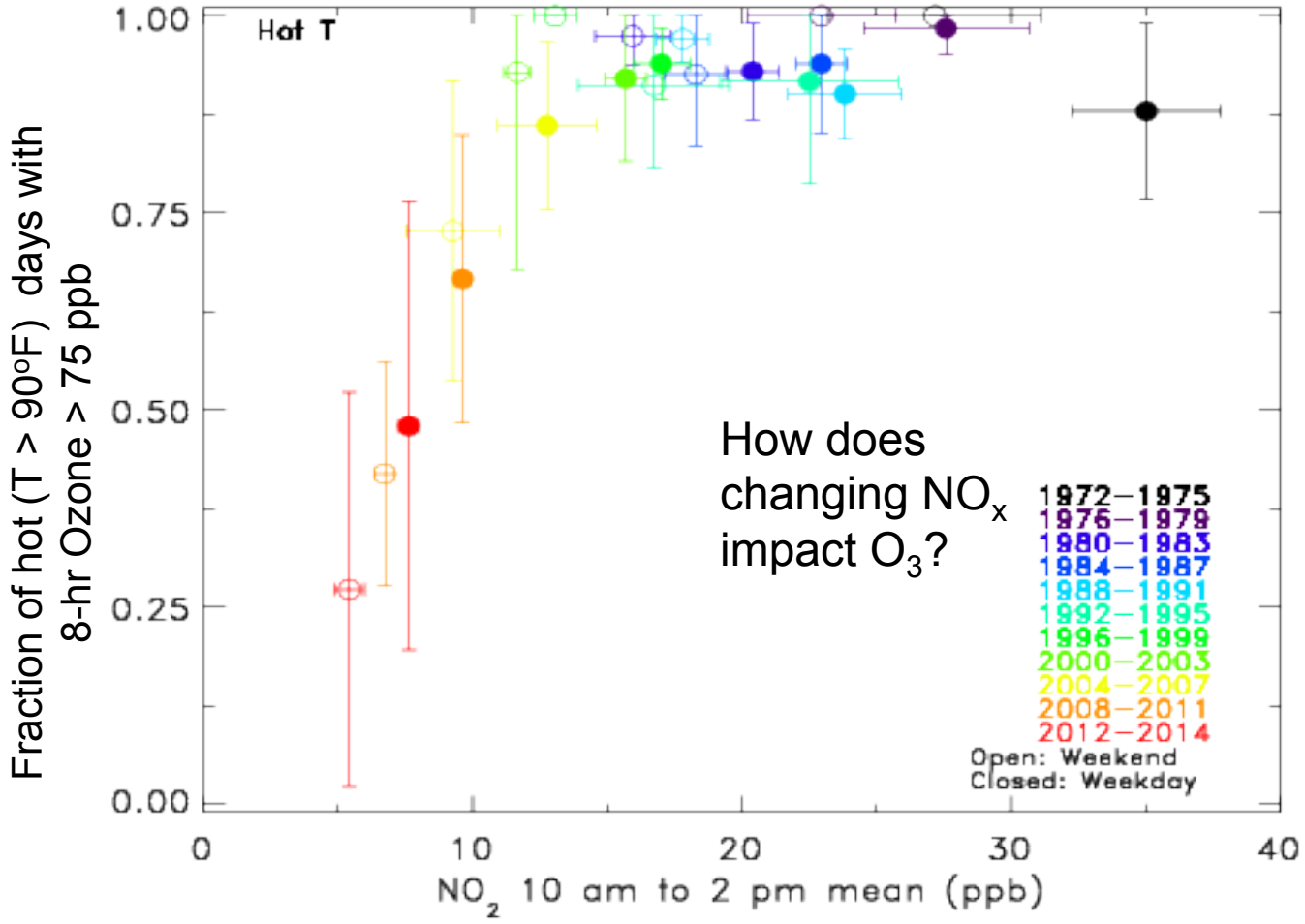

2005
Nitrogen From Space
Satellite Data
NASA
NO_2
1.0e+15
2.0e+15
3.0e+15
4.0e+15
5.0e+15
molecules/cm^2


2011
Nitrogen From Space
Satellite Data
NO2
1.0e+15
2.0e+15
3.0e+15
4.0e+15
5.0e+15
molecules/cm2


Trend in NO_2 from 2005 to 2014 from NASA GSFC
~−2 ppb
−1 ppb
NO_2
-5.0 -4.5 -4.0 -3.5 -3.0 -2.5 -2.0 -1.5 -1.0 -0.5 0.0 0.5
2005-2014 Trend, 10^{15} molecules/cm^2

As measured NO_x levels have gone down …

… *So have ambient ozone levels*

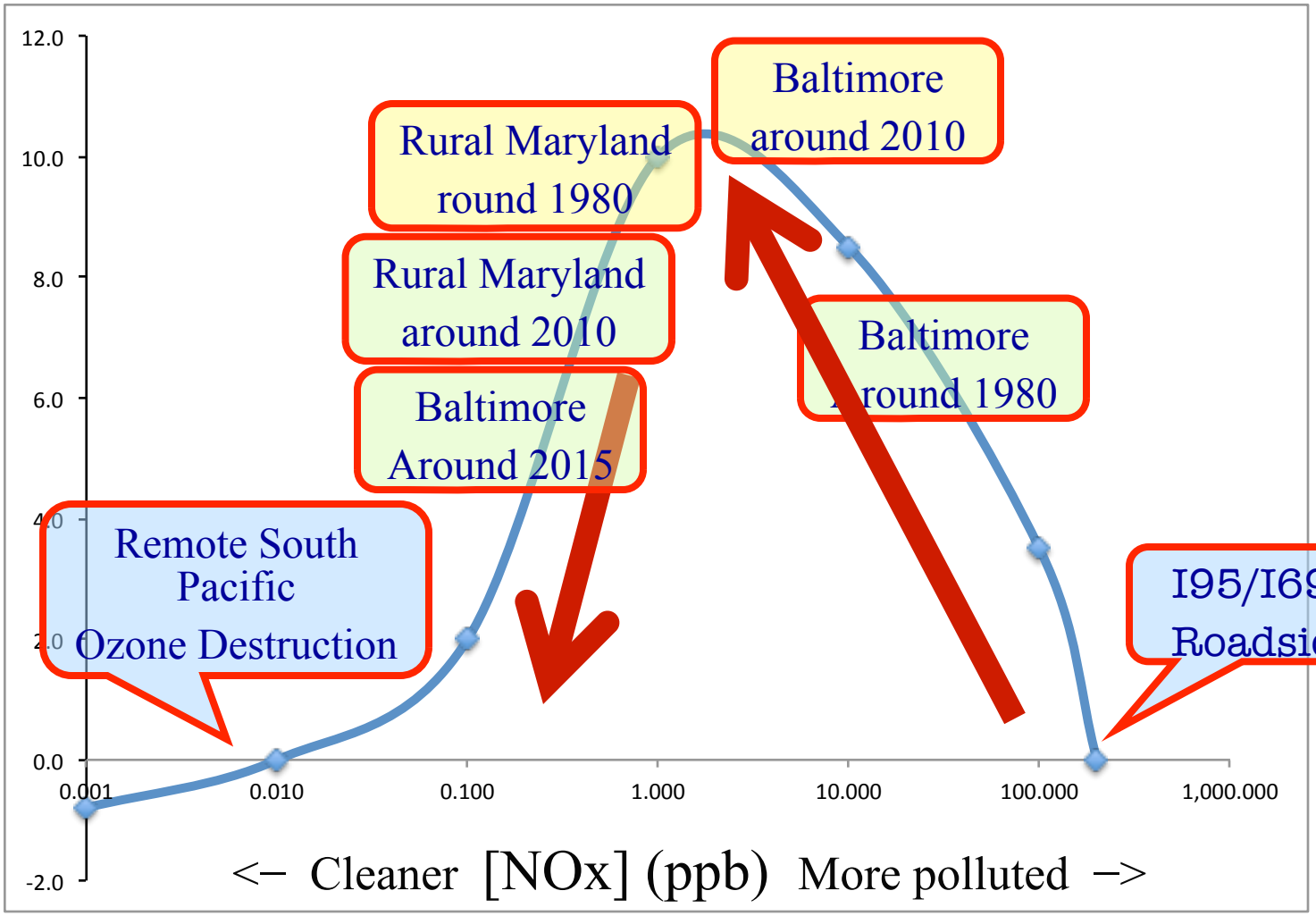


Observations show:
NOx reductions worked, but response is nonlinear;
we had to get over the hump.

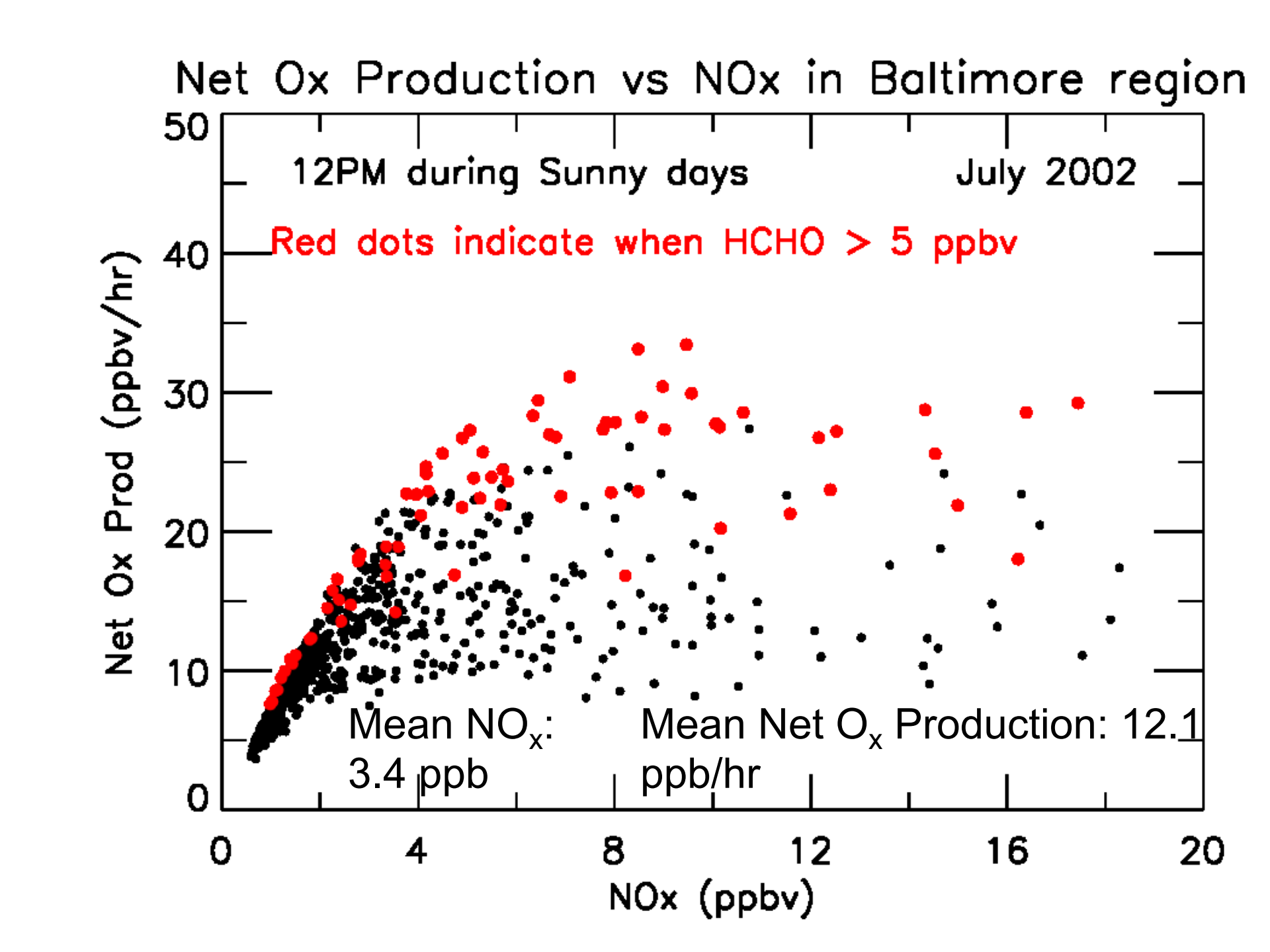
From Goldberg, et al. submitted, 2015.

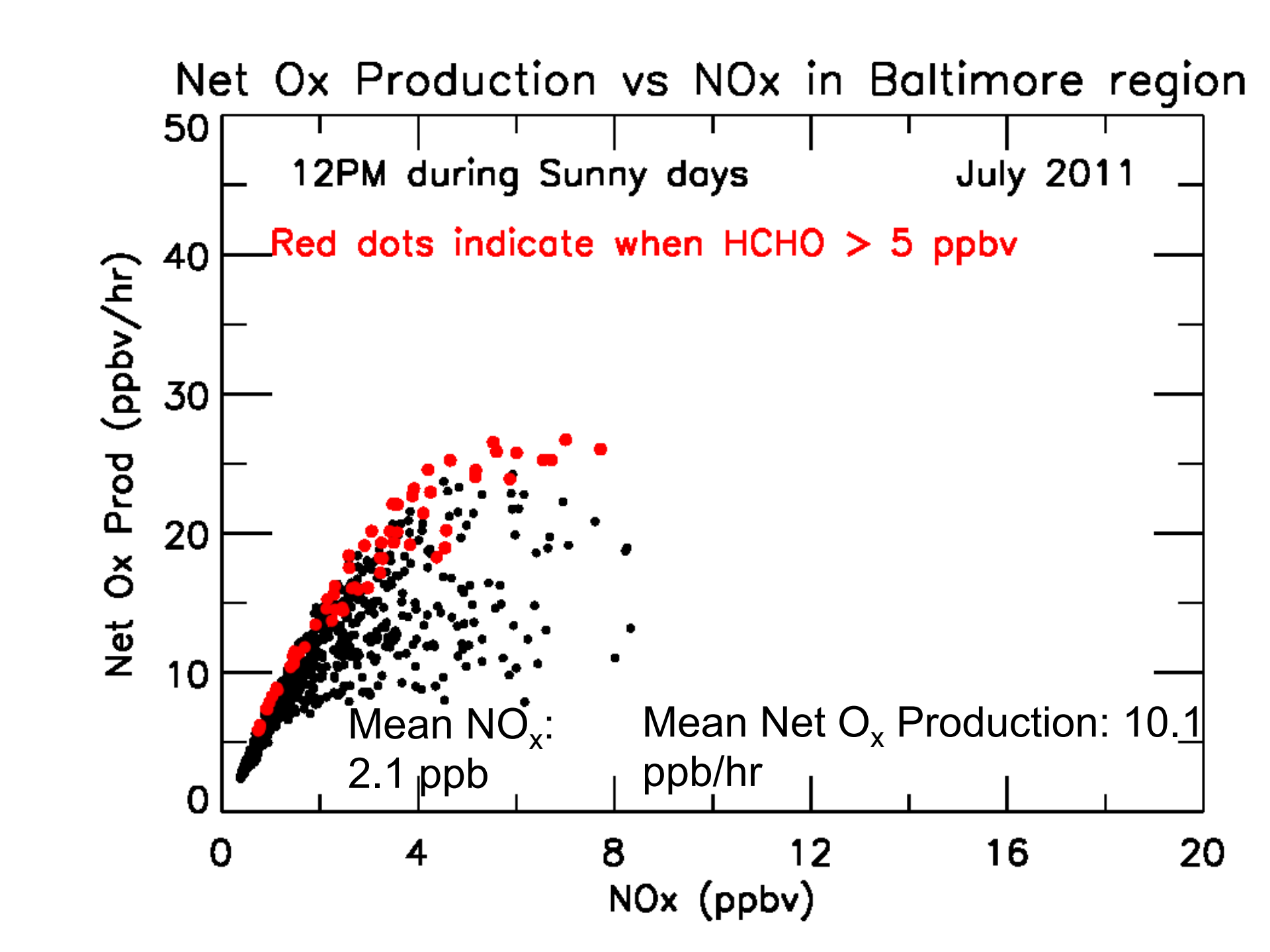
Have We Reached a Tipping Point with NOx?

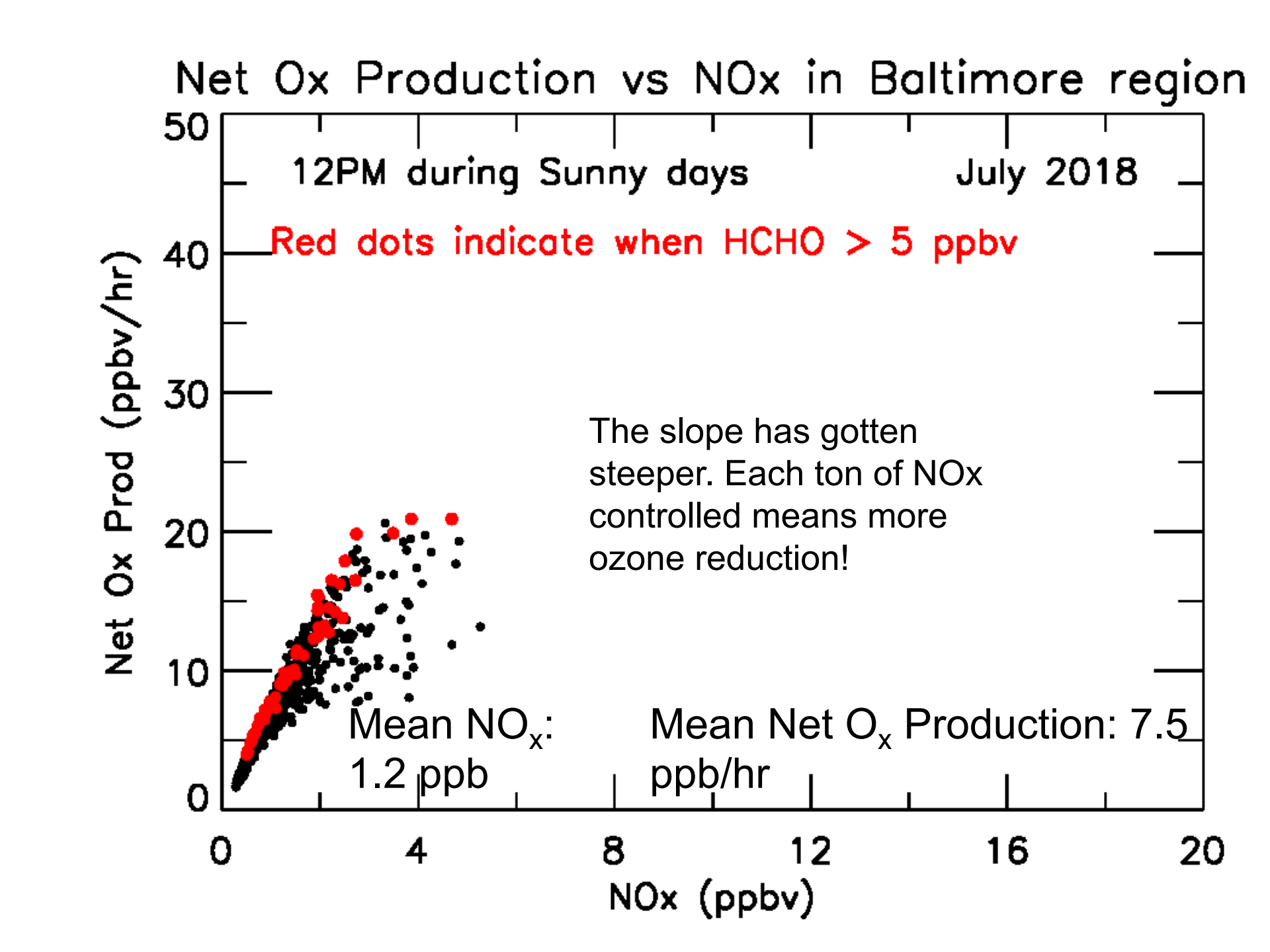
Schematic diagram of ozone production efficiency for the eastern US. - Getting over the hump



MARYLAND
DEPARTMENT OF THE ENVIRONMENT


Net Ox Production vs NOx in Baltimore region
12PM during Sunny days
July 2002
Red dots indicate when HCHO > 5 ppbv
Net Ox Prod (ppbv/hr)
NOx (ppbv)
0
10
20
30
40
50
0
4
8
12
16
20
Mean NOx: 3.4 ppb
Mean Net Ox Production: 12.1 ppb/hr


Net Ox Production vs NOx in Baltimore region
12PM during Sunny days
July 2011
Red dots indicate when HCHO > 5 ppbv
Net Ox Prod (ppbv/hr)
NOx (ppbv)
0
10
20
30
40
50
0
4
8
12
16
20
Mean NOx: 2.1 ppb
Mean Net Ox Production: 10.1 ppb/hr


Net Ox Production vs NOx in Baltimore region
12PM during Sunny days
July 2018
Red dots indicate when HCHO > 5 ppbv
The slope has gotten steeper. Each ton of NOx controlled means more ozone reduction!
Mean NOx: 1.2 ppb
Mean Net Ox Production: 7.5 ppb/hr
Net Ox Prod (ppbv/hr)
NOx (ppbv)
0
10
20
30
40
50
0
4
8
12
16
20

New Science

- Elevated Reservoir
- Sea breezes can exacerbate problems in coastal areas.
- NOx emissions from vehicles are overestimated.
- Biogenic VOC's act as NOx reservoirs and expand the area for ozone production.

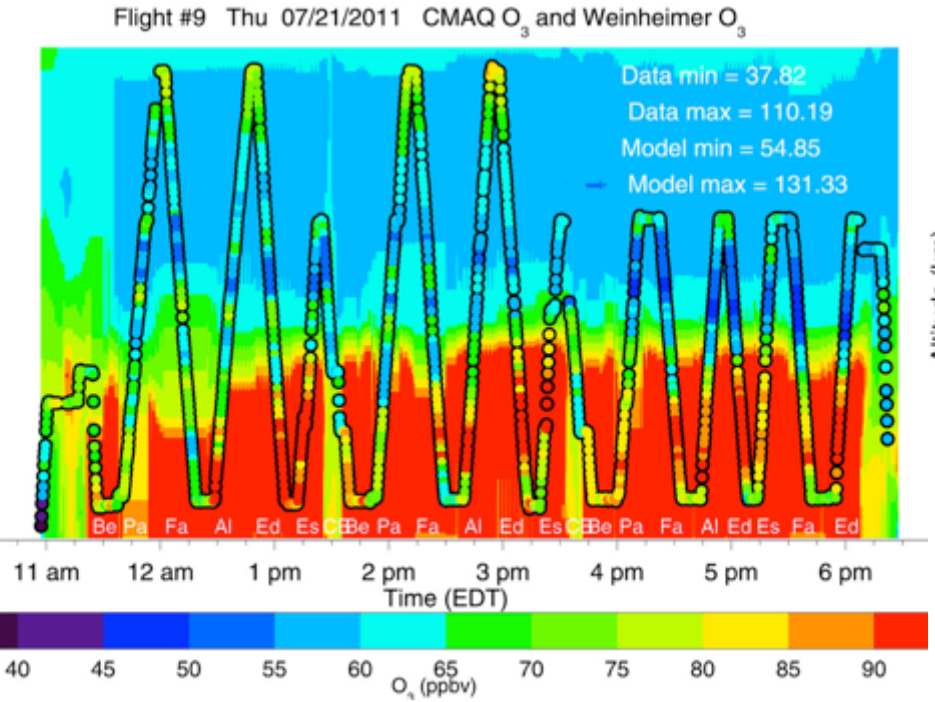
The Aloft Reservoir

Much of the transport of smog is in the LFT.

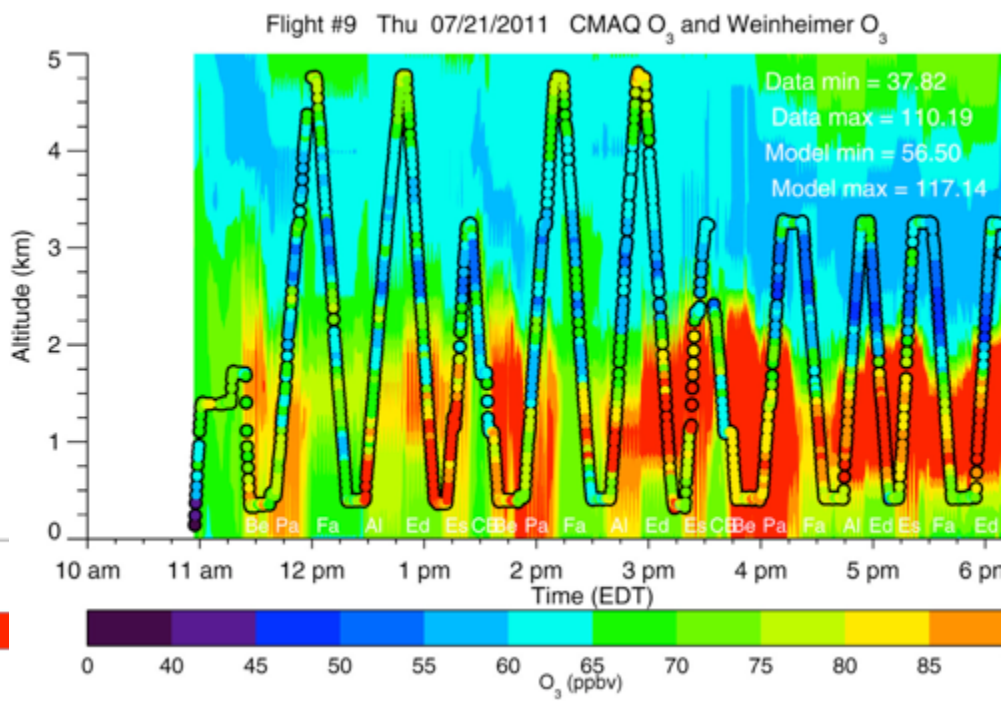
CMAQ with 12 km resolution cannot resolve the elevated O_3 reservoir of ozone, but with 4 km it can. Important to NOAA/ARL AQ forecast.

He et al., *Atmos. Environ.*, 2014

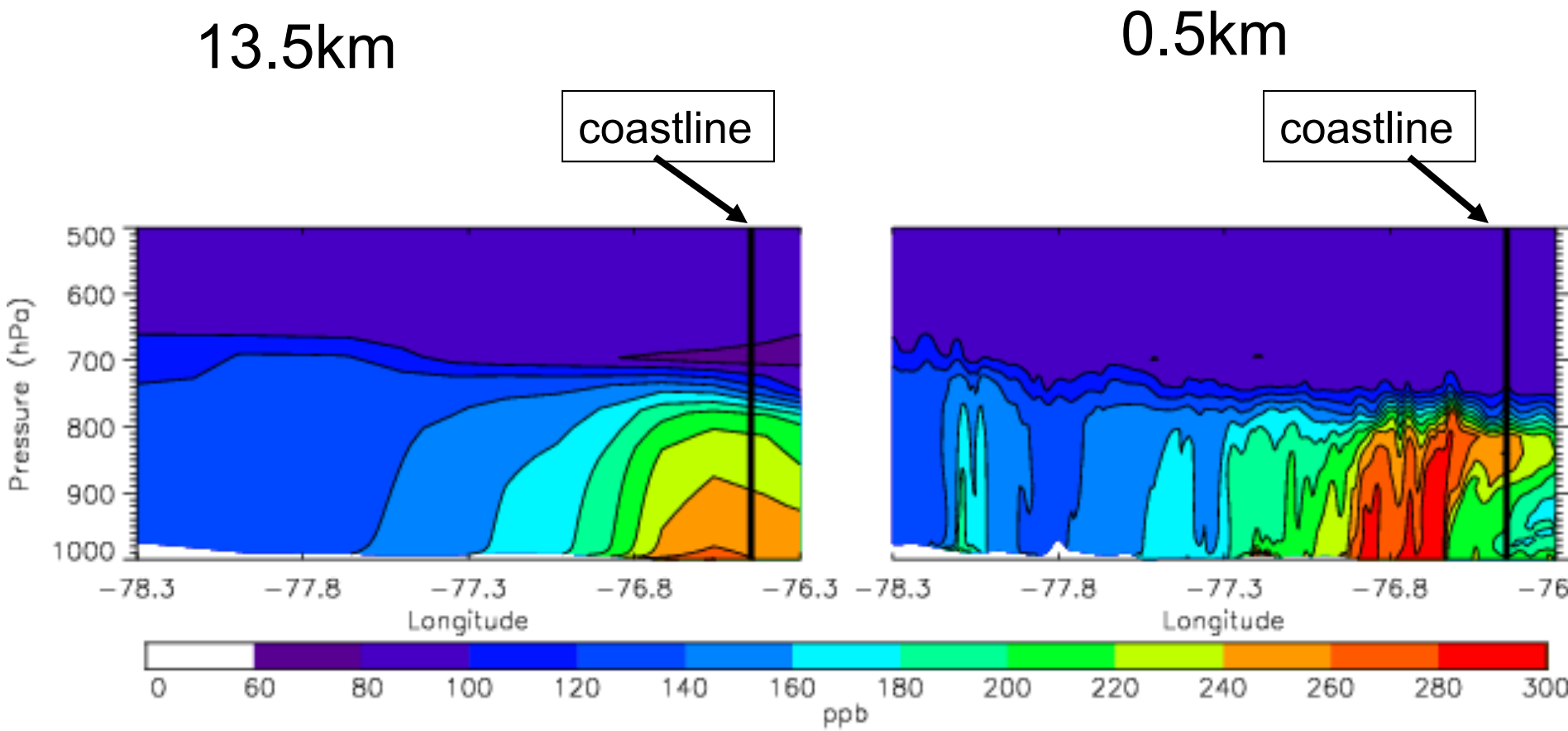
12 km CMAQ ↓



4 km CMAQ ↓



Cross-section of CO between Washington, DC and Baltimore, MD for the 13.5 and 0.5 km simulations. The stronger bay breeze in the 0.5 km simulation causes higher concentrations at the convergence zone leading to lofting and downwind transport.



Summary

- We have made great progress on understanding the science behind ozone in the eastern US and improving AQ, but *miles to go before we sleep.*
- We will continue to work with MDE, NASS, NOAA, EPA,& OTC and expand focus to include CT/NY.
- What will remain constant is NOx controls work.

The End

WANT to get more NASA help?

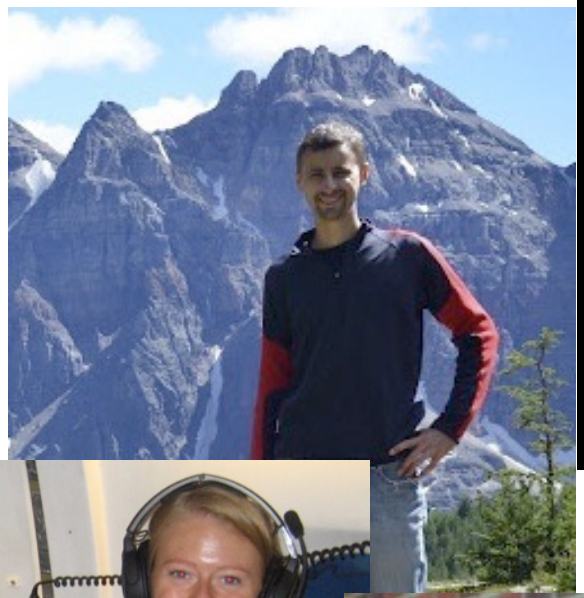
Write Drs. Michael Freilich
&, Jack Kaye
NASA Headquarters
Earth Science Programs,
300 E St SW, Washington,
DC 20546

Fear the Turtle!

Reprints can be found at http://www.atmos.umd.edu/~russ/recent_pubs.html

Backup Slides

The Guilty Parties






When measurements and CTMs disagree:

- Dispersion could be wrong.
- Emissions could be wrong.
- Chemistry (formation, sequestering, or removal) could be wrong.
- Some combination of the above.

Let's look at ratios

- EPA inventories estimate a NO_y/CO ratio of ~136 mmol/mol (CO/NOx ~ 7-9).
- Previous research suggests inventory ratios of NO_y/CO are an overestimate:
  - Fujita (2012) – models overestimate concentrations by 25-40%
  - Parrish (2006) – Inventories are a factor of 2 larger than measurements
- Research questions:
  - What are the emissions ratios of pollutants NO_y & CO Maryland?
  - How well do emissions inventories represent these ratios?

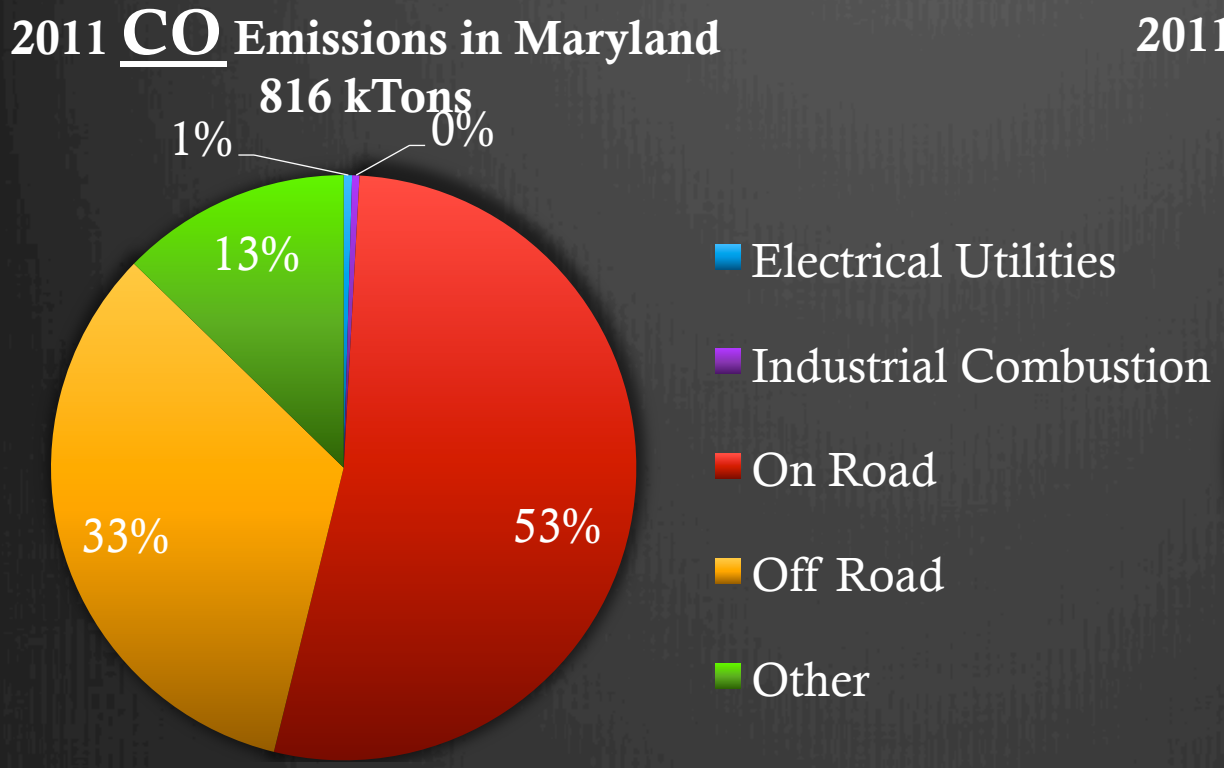
* NOy = NOx + products HNO_3, PAN, $RONO_2$, NO_3^-

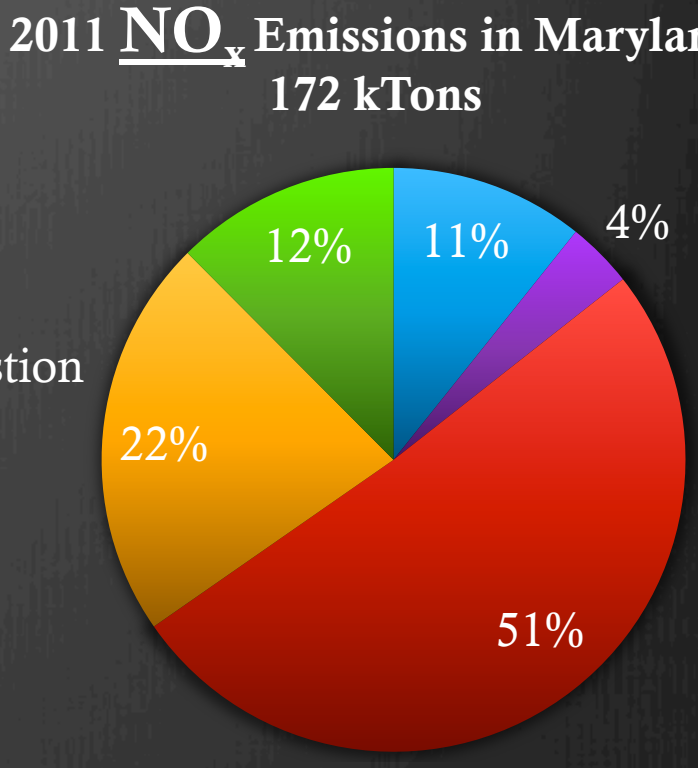
Methodology

- Identified 70 spirals from DISCOVER-AQ P3B flights with simultaneous peaks and areas of correlated CO and NO_y concentration.
- Determined mixed layer from vertical profiles of relative humidity and equivalent potential temperature.
- Calculated, for measured compounds in the mixed layer, $\Delta NOy/\Delta CO_2$ and $\Delta NOy/\Delta CO$.
- Included only those correlations with $r^2 > 0.8$ and with > 10 data points.
- Average plume age ~ 3 hr.

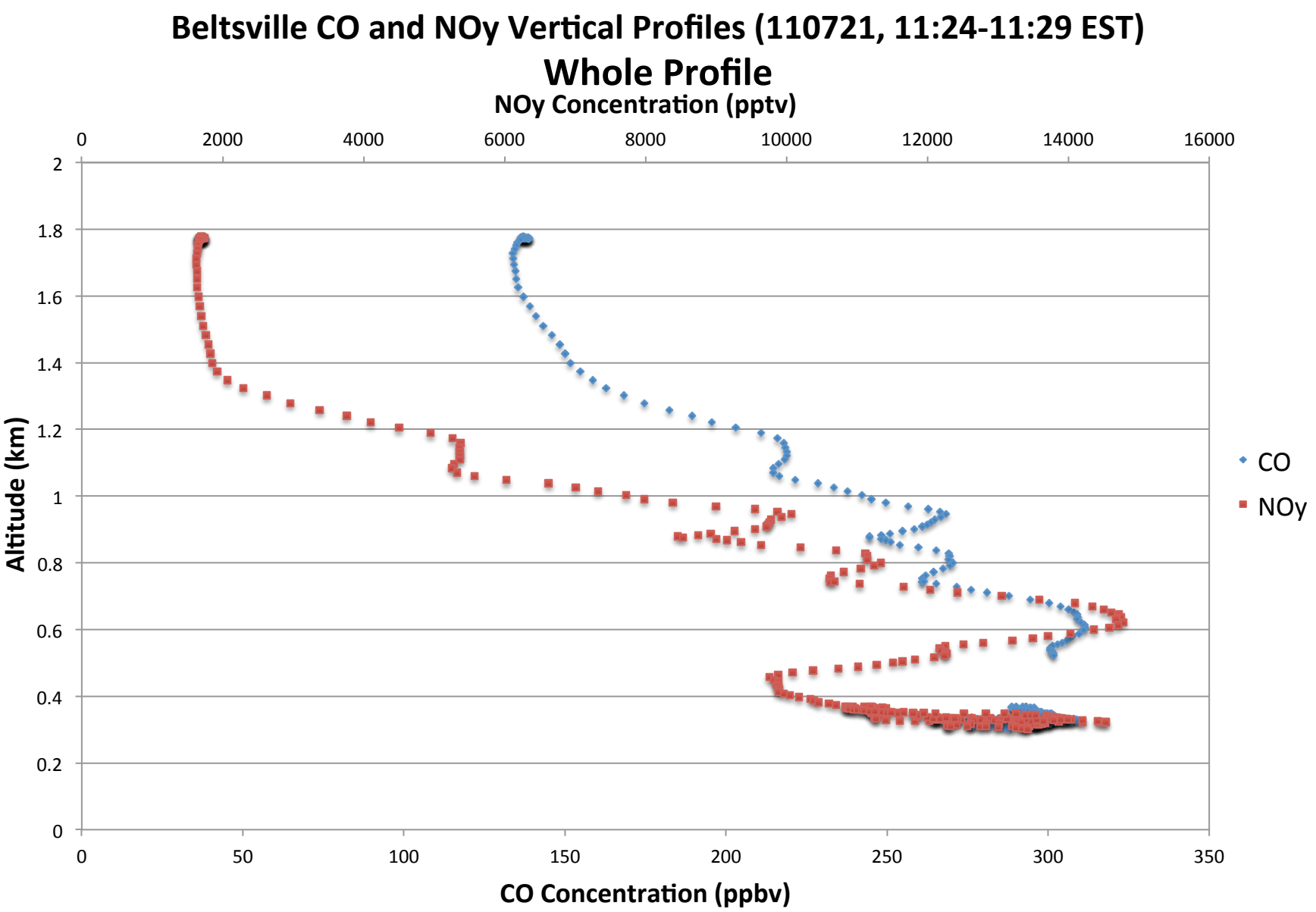
Anderson et al., *Atmospheric Environment*, 2014.

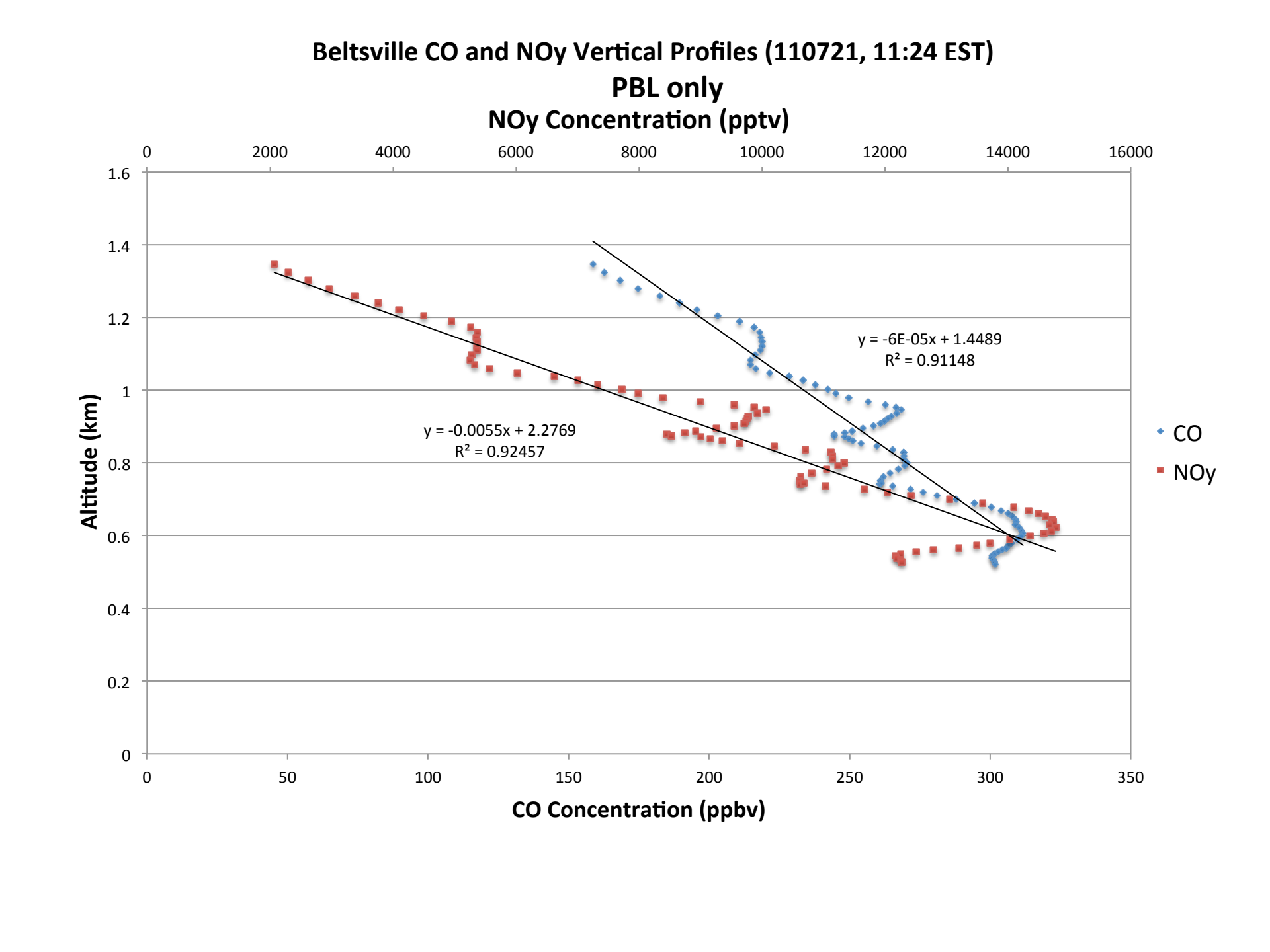
From NEI





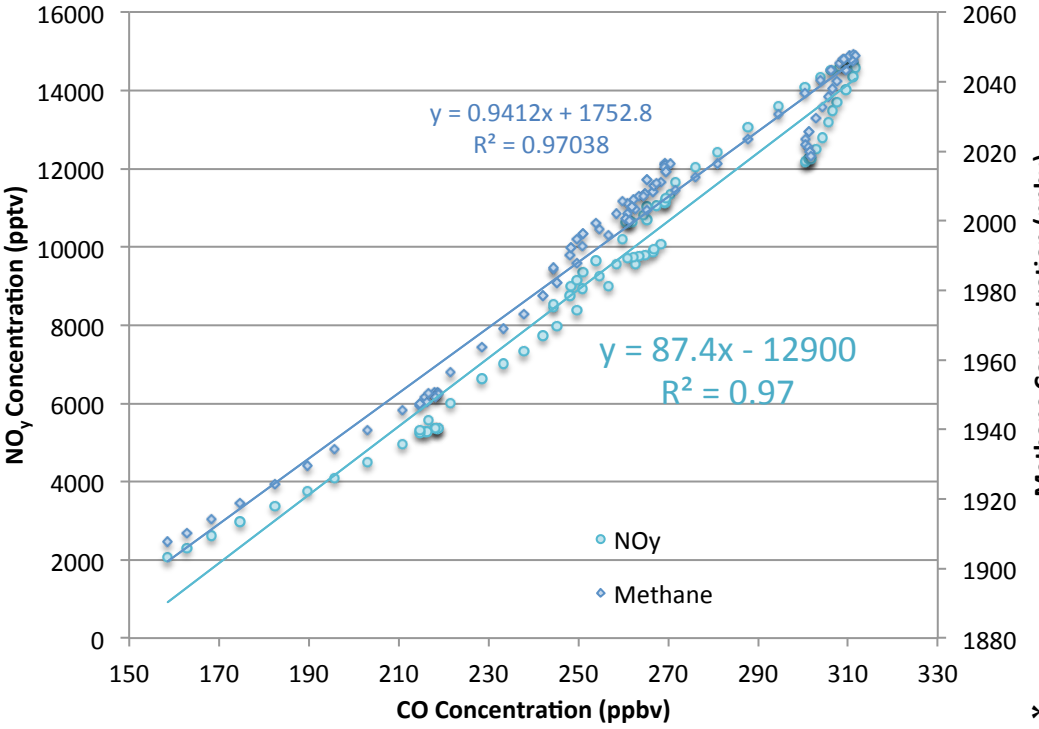
- CO and NO_x are important O_3 precursors.
- Significant disagreement among studies on NEI's accuracy.
- Can we use *in situ* observations to evaluate these numbers?

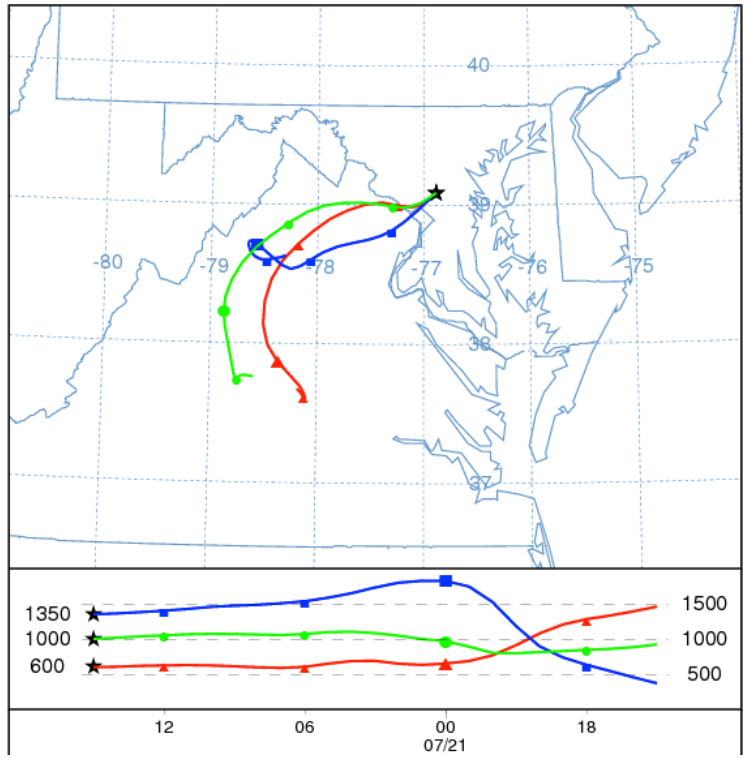

Beltsville CO and NOy Vertical Profiles (110721, 11:24-11:29 EST)
Whole Profile
NOy Concentration (pptv)
0
2000
4000
6000
8000
10000
12000
14000
16000
Altitude (km)
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
CO Concentration (ppbv)
0
50
100
150
200
250
300
350
CO
NOy


Beltsville CO and NOy Vertical Profiles (110721, 11:24 EST)
PBL only
NOy Concentration (pptv)
0
2000
4000
6000
8000
10000
12000
14000
16000
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Altitude (km)
y = -6E-05x + 1.4489
R² = 0.91148
y = -0.0055x + 2.2769
R² = 0.92457
CO
NOy
0
50
100
150
200
250
300
350
CO Concentration (ppbv)

Beltsville, 110721, 868-953 hPa, 11:27 EST

Air mass from DC and Virginia.
NO_y/CO ratio ~0.087 or CO/NOy = 11.5

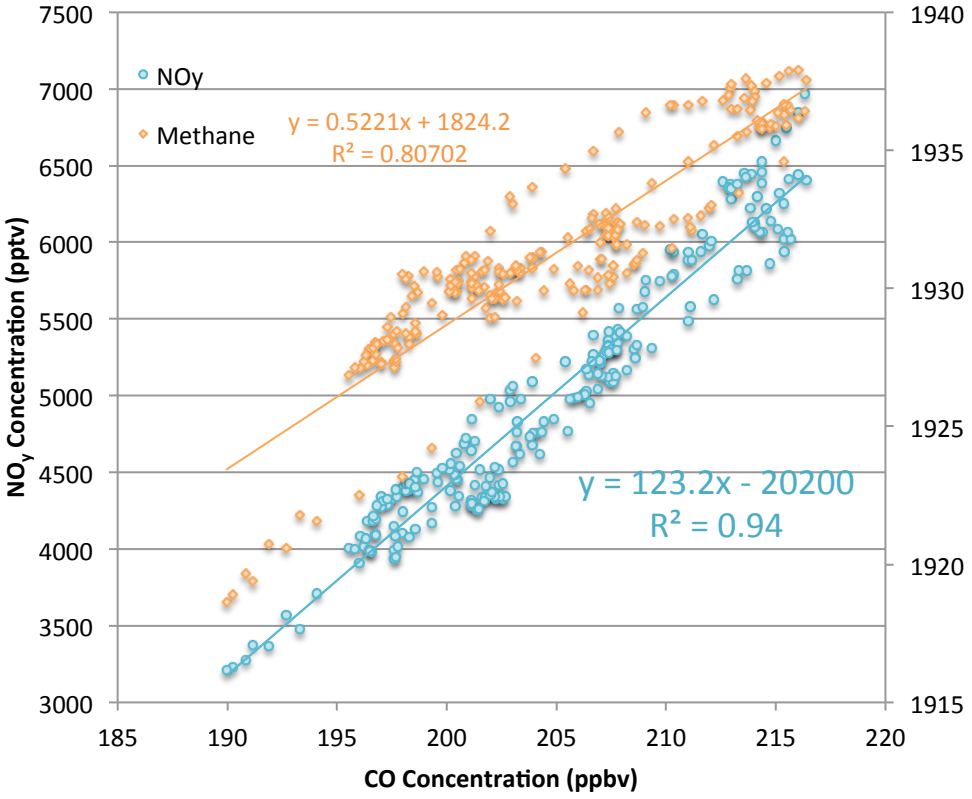


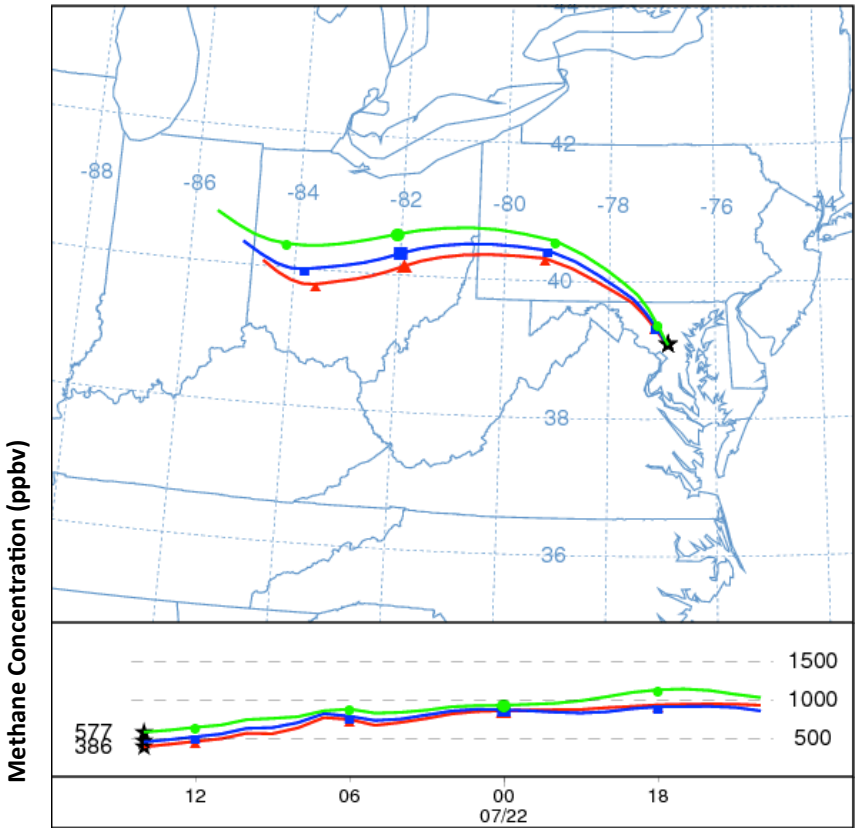


Preliminary Data. Do not cite.

Beltsville, 110722, 949-979 hPA, 10:05 EST

Air mass from Ohio River Valley.
NO_y/CO ratio slightly higher (123) or CO/NOy lower (8.0) than previous profile.

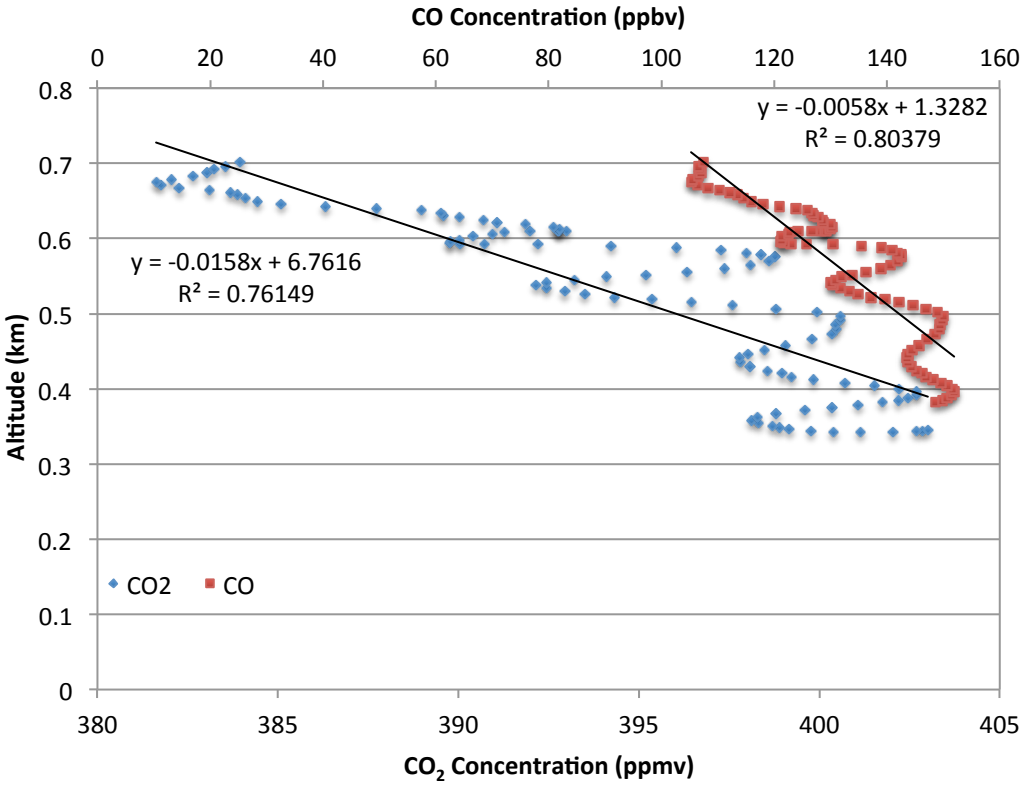


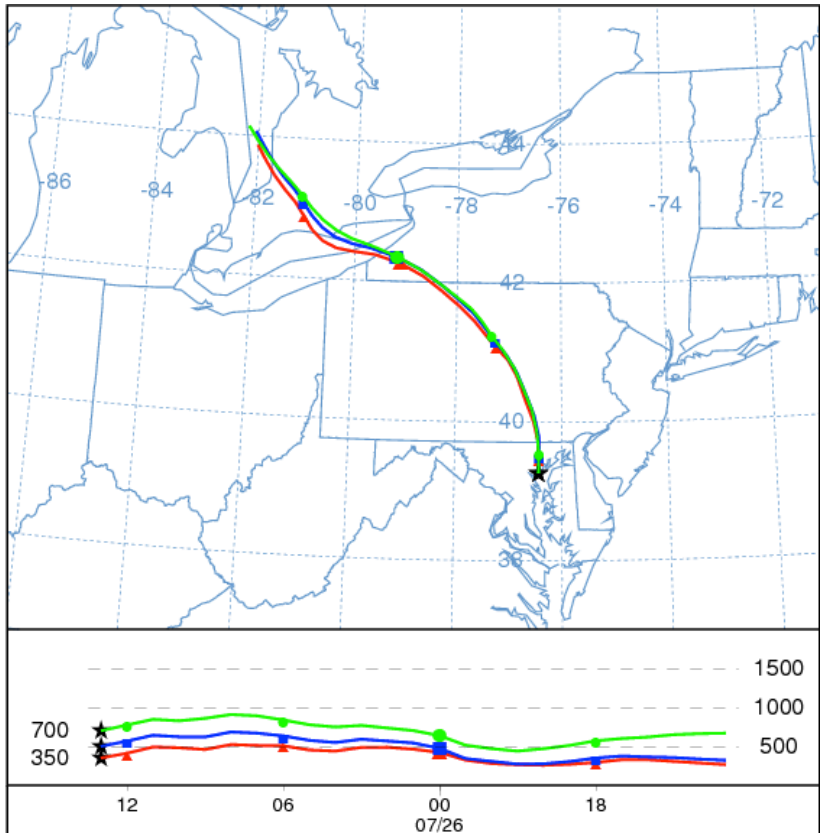


Preliminary Data. Do not cite.

Essex, 07/26, 9:13 EST

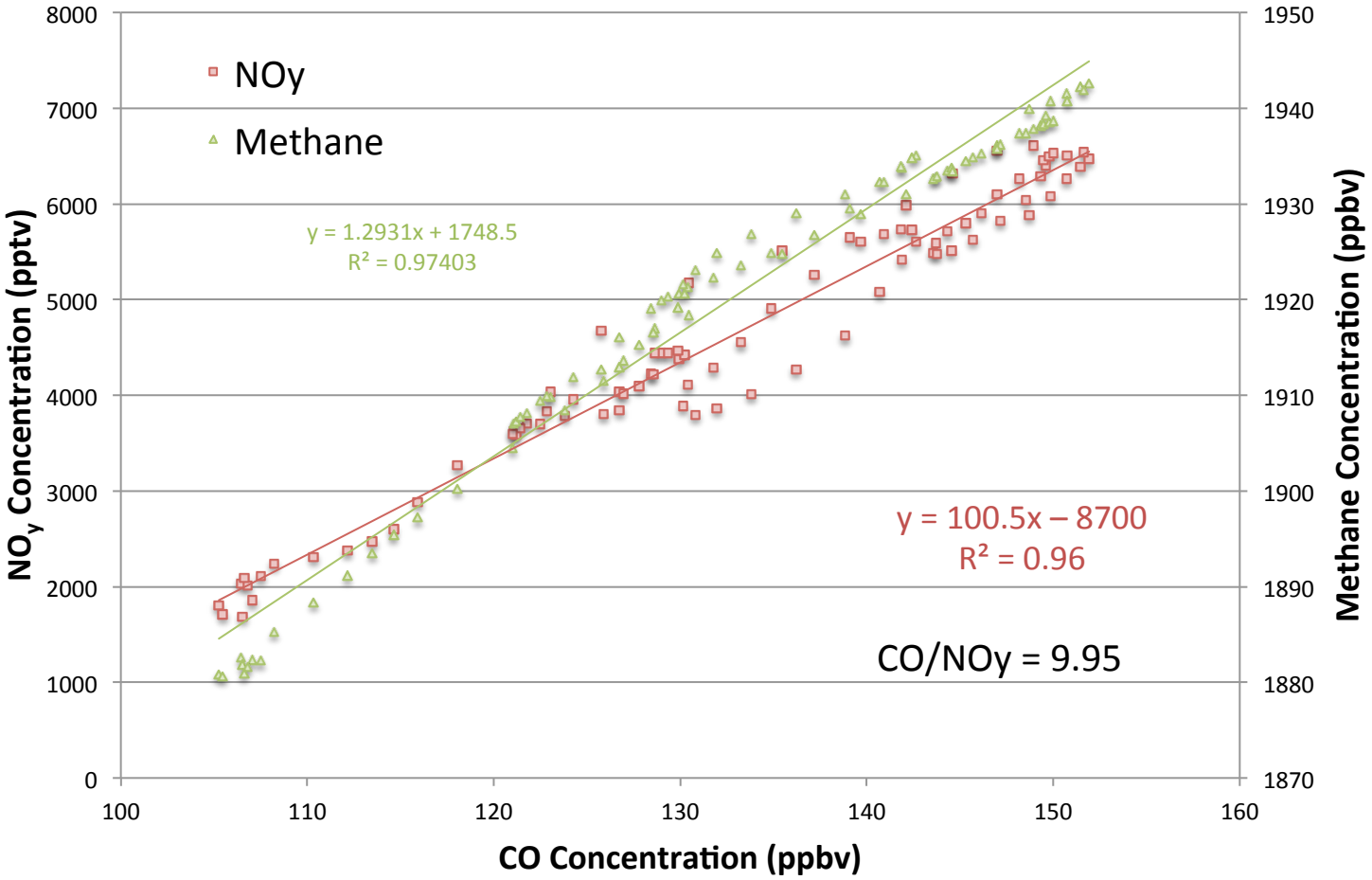
Portion of vertical profile in the mixed layer:





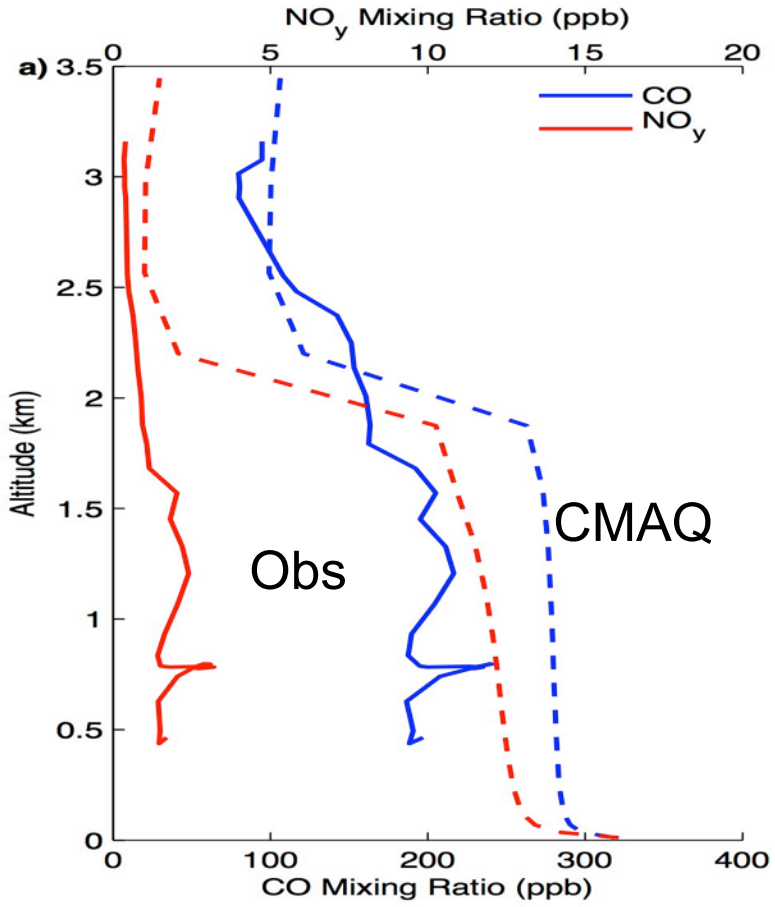
Air mass from "clean corridor" in PA. Pollution probably local.

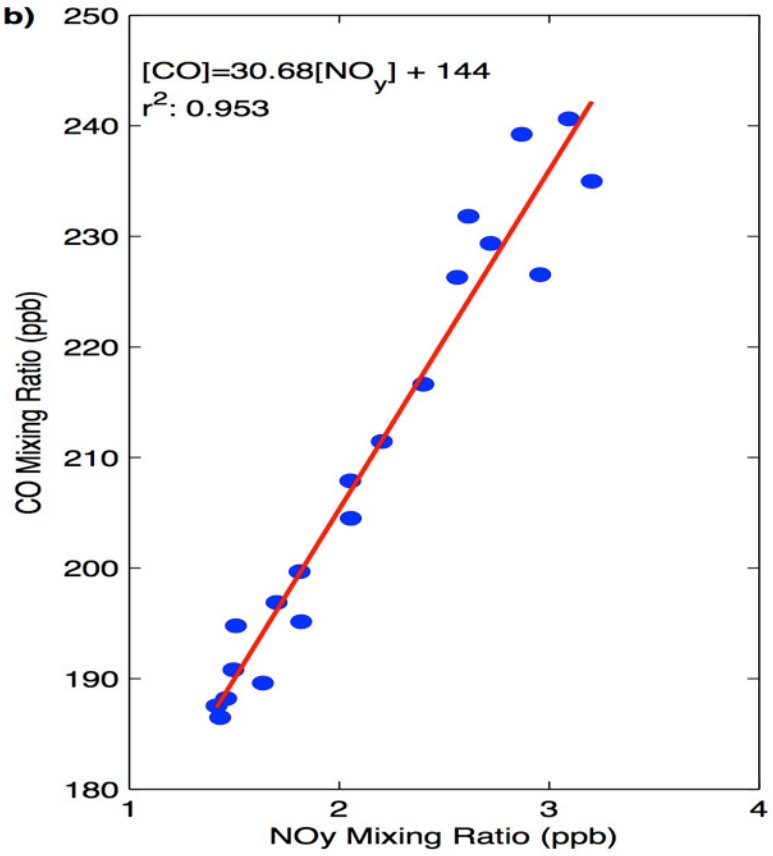
Essex, **07/26, 9:13 EST**



Anderson et al. *Atmos. Environ.*, 2014.

CO/NOy ratios in CMAQ are higher than observed.
Padonia 11 July 2011





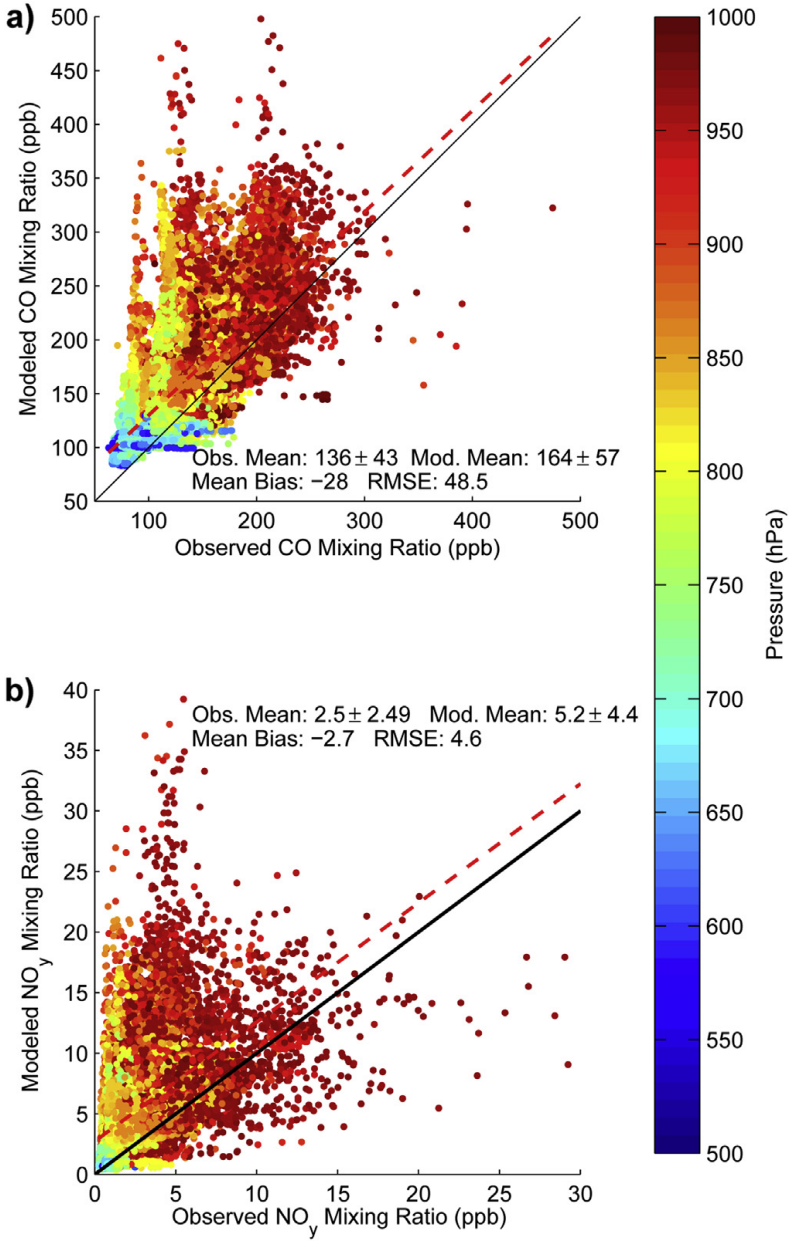
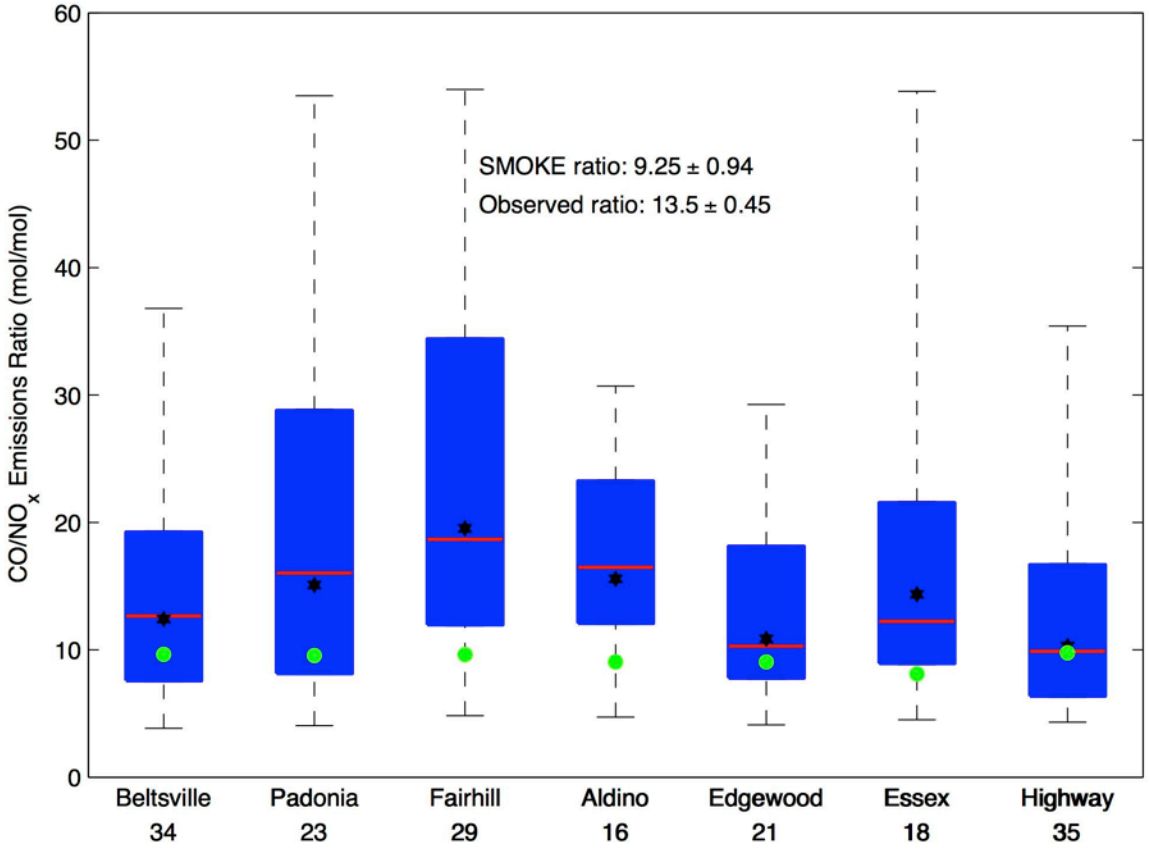


Fig. 7. a) Regression of measured and modeled CO for all flight days during DISCOVER-AQ. Values after means are 1σ. b) Same as a) but for NO_y. Solid line is the 1:1 line; dashed line, the line of best fit.

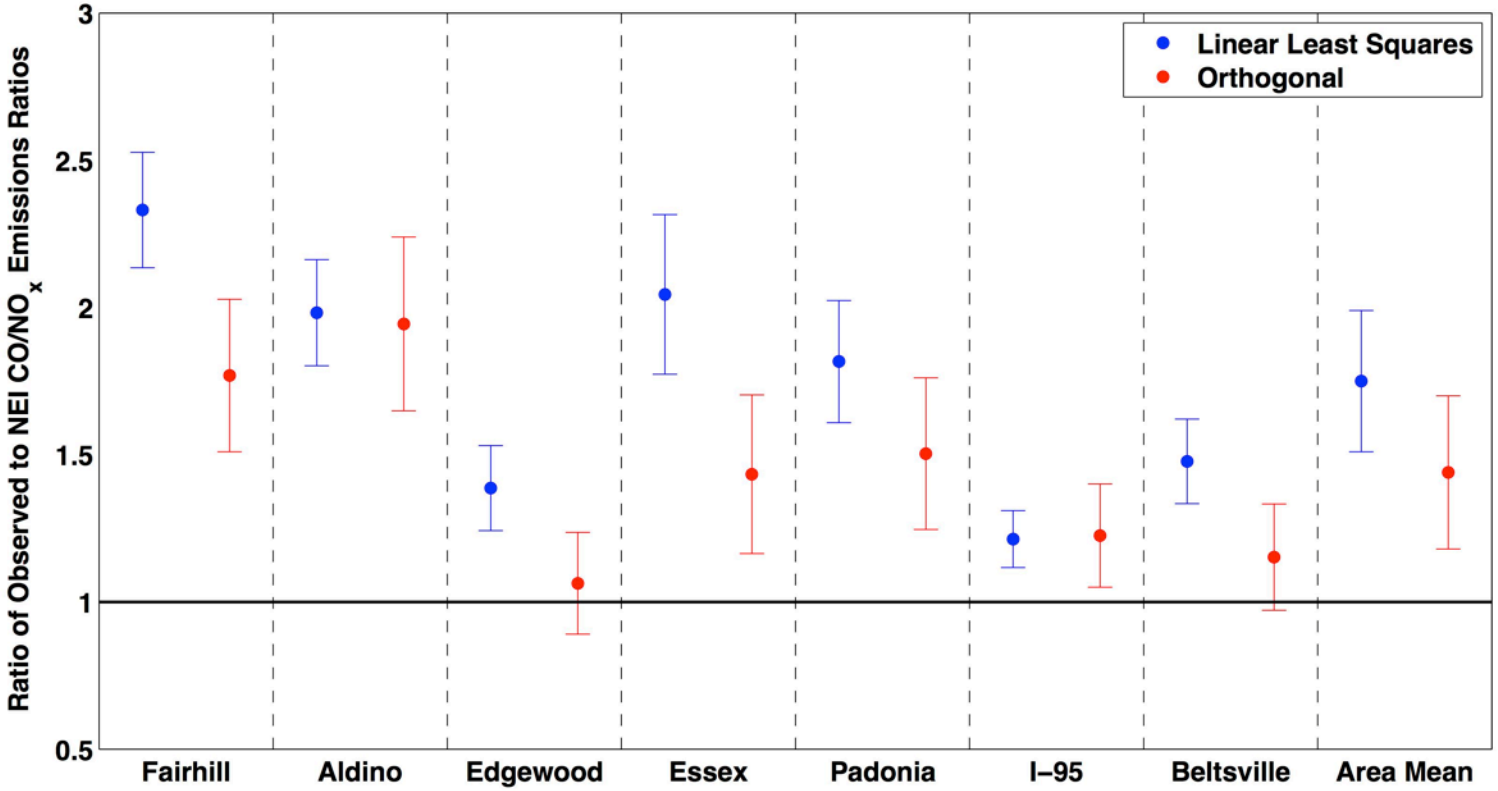
CMAQ gets CO a little high (bias = +28 out of 136 ppb) but NOy much too high (bias +2.7 out of 2.5 ppb).

Summary of Results

CMAQ/CB05 gets CO about right (15 ±11% high), but substantially overestimates NOy.



Evaluation of NEI NO_x Emissions



- NEI overestimates NO_x emissions by 40-75%.
- MOVES likely underestimates the lifetime & efficiency of catalytic converters.
- Is the driving cycle right?

Summary of Emissions Ratios

	DISCOVER-AQ Average (mol/mol) ± $\sigma/n^{0.5}$	Number of aircraft profiles	Fujita *et al* 2012 (mol/mol)	EPA (mol/mol)	EPA/ DISCOVER-AQ
CO/NOy	**13.7 ± 1.4**	**60**	**9.3**	**7.4+**	**0.54**

*: Values for 2010 +: Values for 2011; CO & NO_y data from NEI.

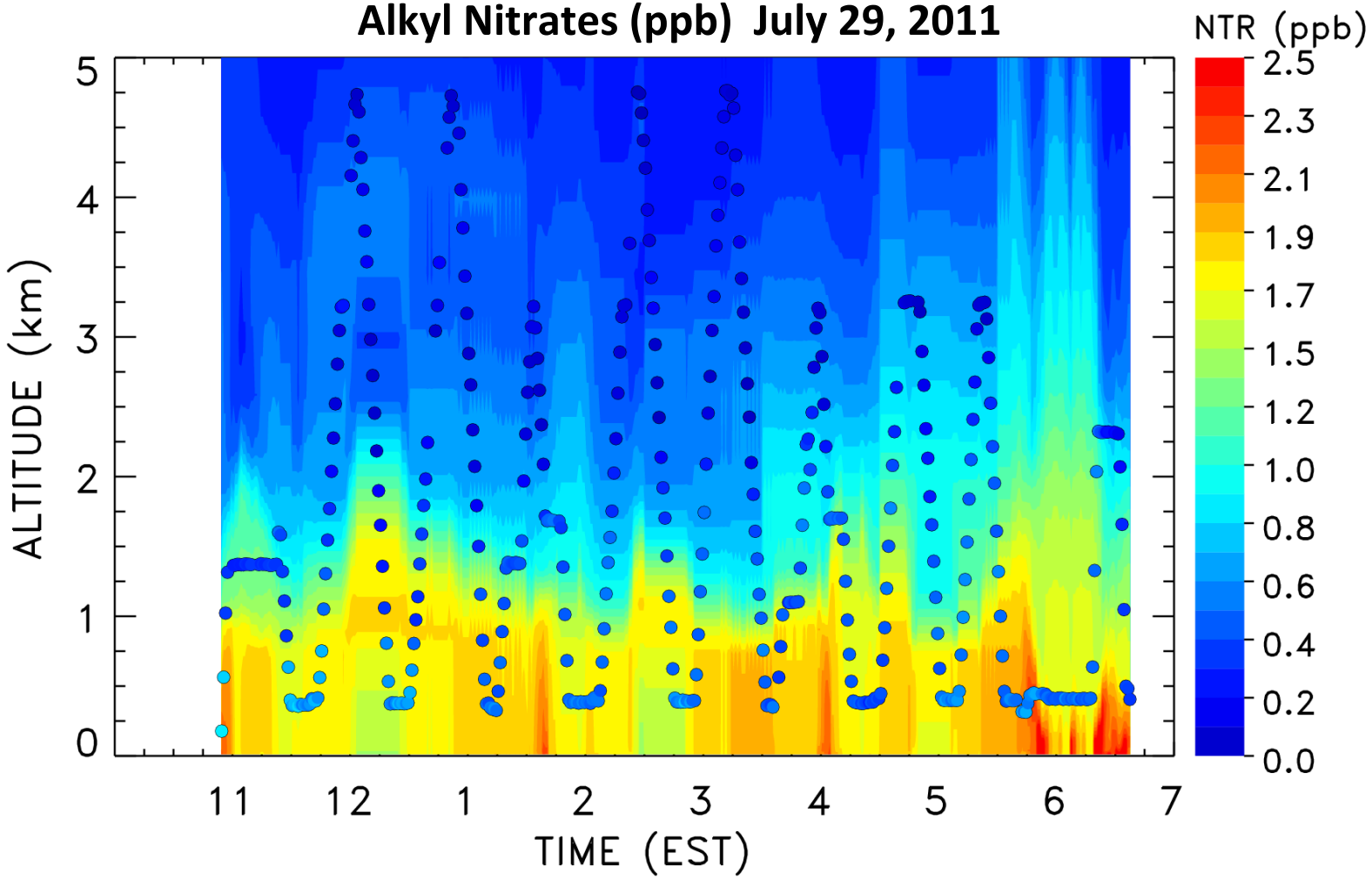
NEI appears to overestimate NOx emissions by a factor of ~2.

Anderson et al., Atmos. Environ., 2014.

What impact does reduced NOx emissions have on model performance?

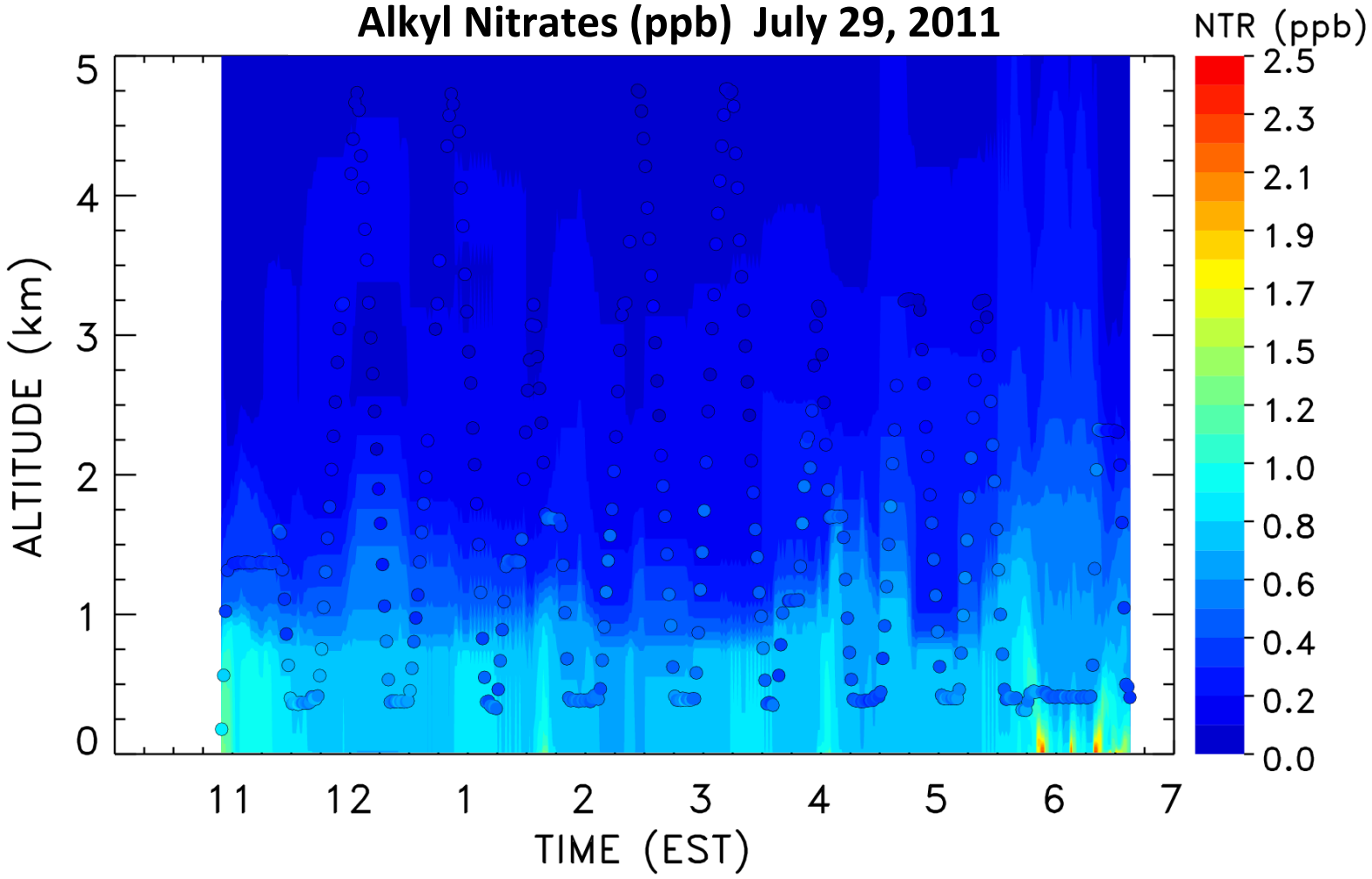
- Do we get O_3 right for the wrong reasons?
- Alkyl nitrates (AN), including isoprene nitrates, represented as single species (NTR).
- We can compare aircraft observations during DISCOVER-AQ to CMAQ model run for 2011.
- With CMAQ "off the shelf" NTR overestimated.

From Canty et al., *ACP*, 2015.



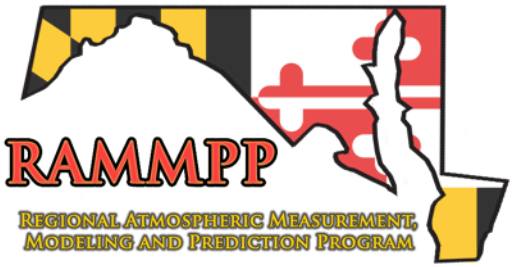
Background Contour → CMAQ Baseline

Colored points → DISCOVER-AQ Flight #14



Background Contour → CMAQ decreased AN lifetime, 50% ↓ mobile NO_x
Colored points → DISCOVER-AQ Flight #14

Has this been seen before?



Houston - EPA RTP guys [*Yu et al.*, 2012]

Compares CMAQ (WRF; CB4.2; Mobile 6 and BEIS) to the TEXaqs 2006 observations. They conclude:

Compared to P3 obs in the lowest 200m, the model:

- Does well for CO (124 observed vs. 117 ppb modeled)
- Does well for O_3.
- **Overestimates NOy (9.2 vs. 4.6 ppb) and all NOy constituents.**
- Shows the OPE substantially less than observed from O_3 vs. NOz (8 vs. 3).

Yu, S. C., et al. (2012), Comparative evaluation of the impact of WRF-NMM and WRF-ARW meteorology on CMAQ simulations for O_3 and related species during the 2006 TexAQS/GoMACCS campaign, *Atmospheric Pollution Research, 3*(2), 149-162.