Recent Ozone Modeling Results

Presentation by:
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Modified for AQAST, September 25, 2015

UNIVERSITY OF MARYLAND

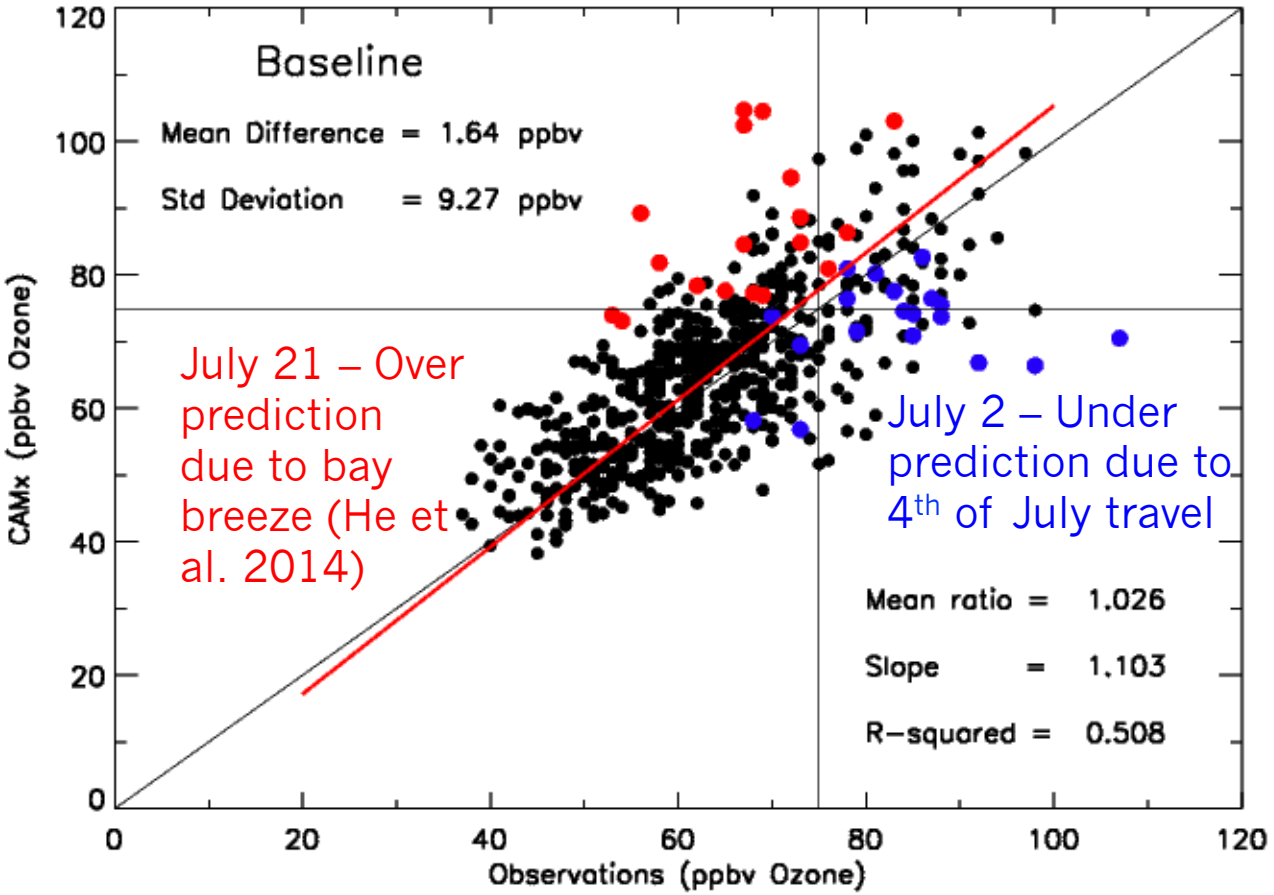
MDE

Description of model used:

- CAMx v6.10 (12 km OTC model domain)
  - EPA-approved regulatory model
  - Can use the *CB6r2* gas-phase chemical mechanism (Ruiz & Yarwood, 2013)
    - Better alkyl nitrate chemistry
  - Ability to use ozone source apportionment technology (*OSAT*) to identify where the ozone "originated" by region & sector

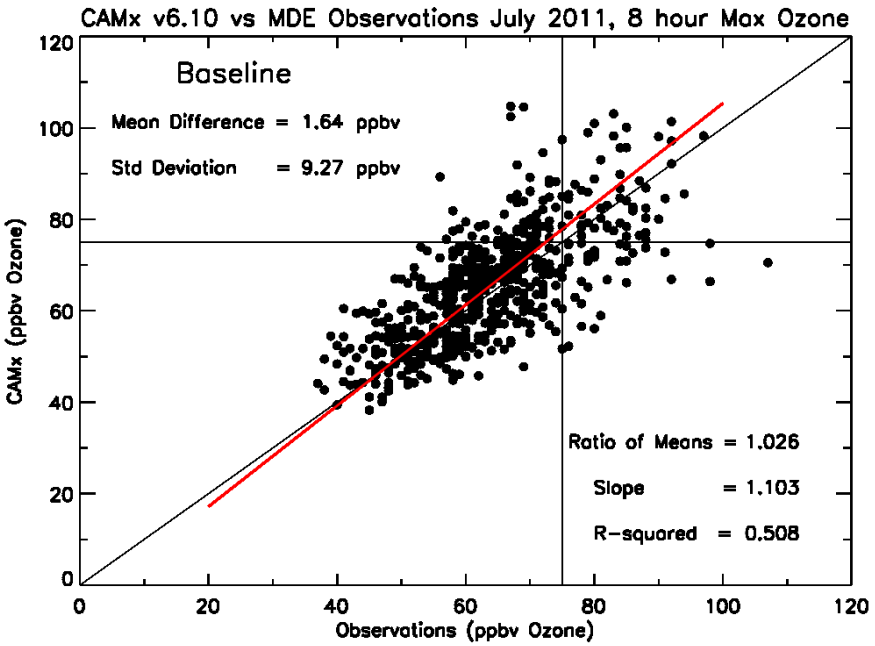
Model Verification

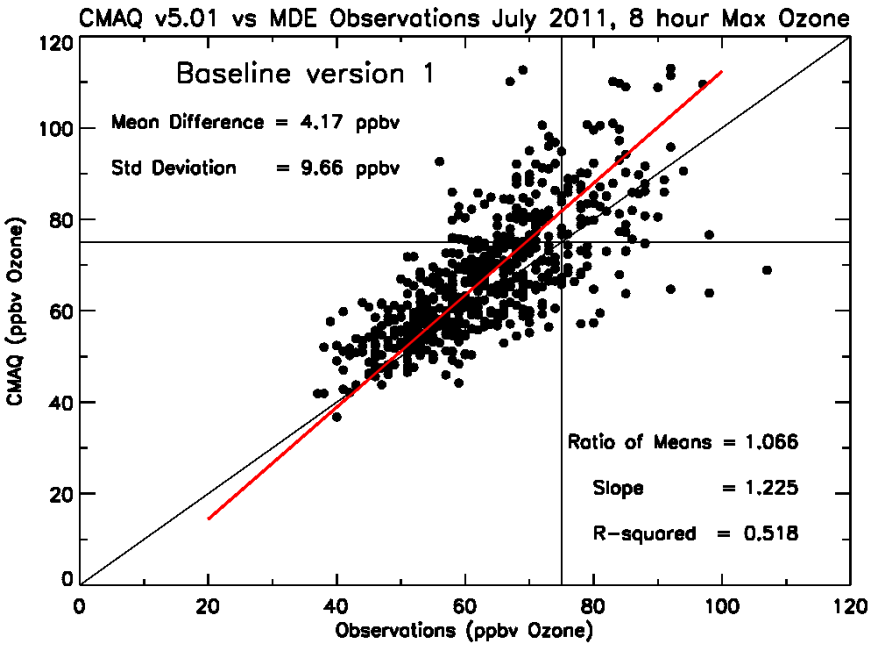
July 2011 8-hour maximum surface ozone: CAMx model vs. observations in Maryland



There is **excellent** model agreement in predicting *monthly surface* ozone when using the standard, "off-the-shelf" version of CAMx

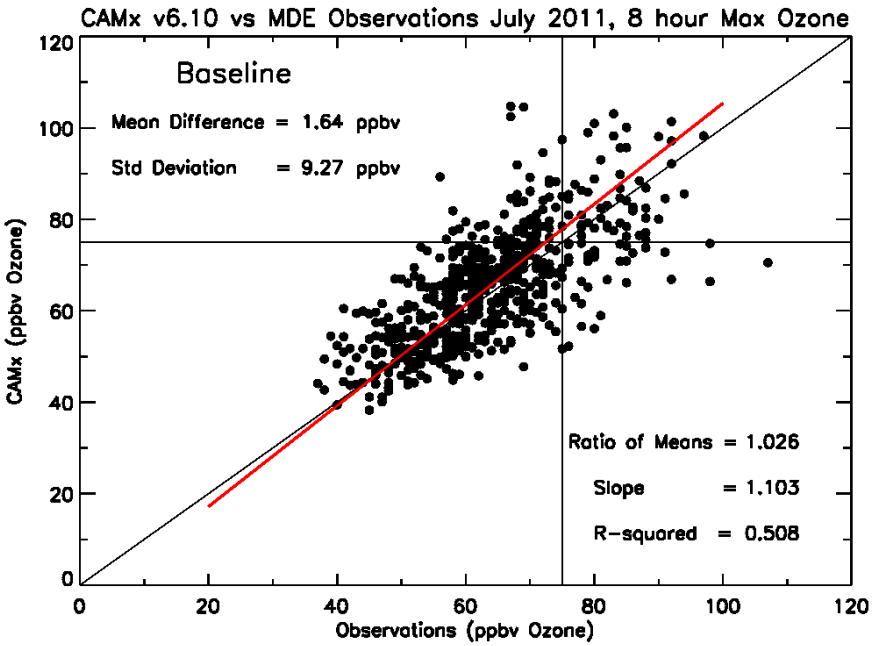
Models compared to observations

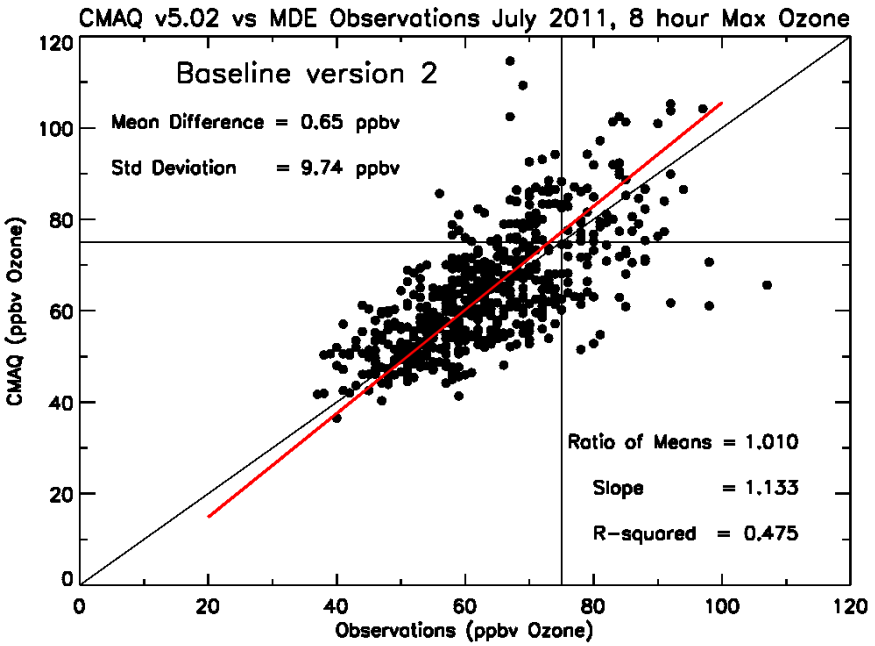




- CAMx performs slightly better at predicting surface ozone using version 1 of the emissions

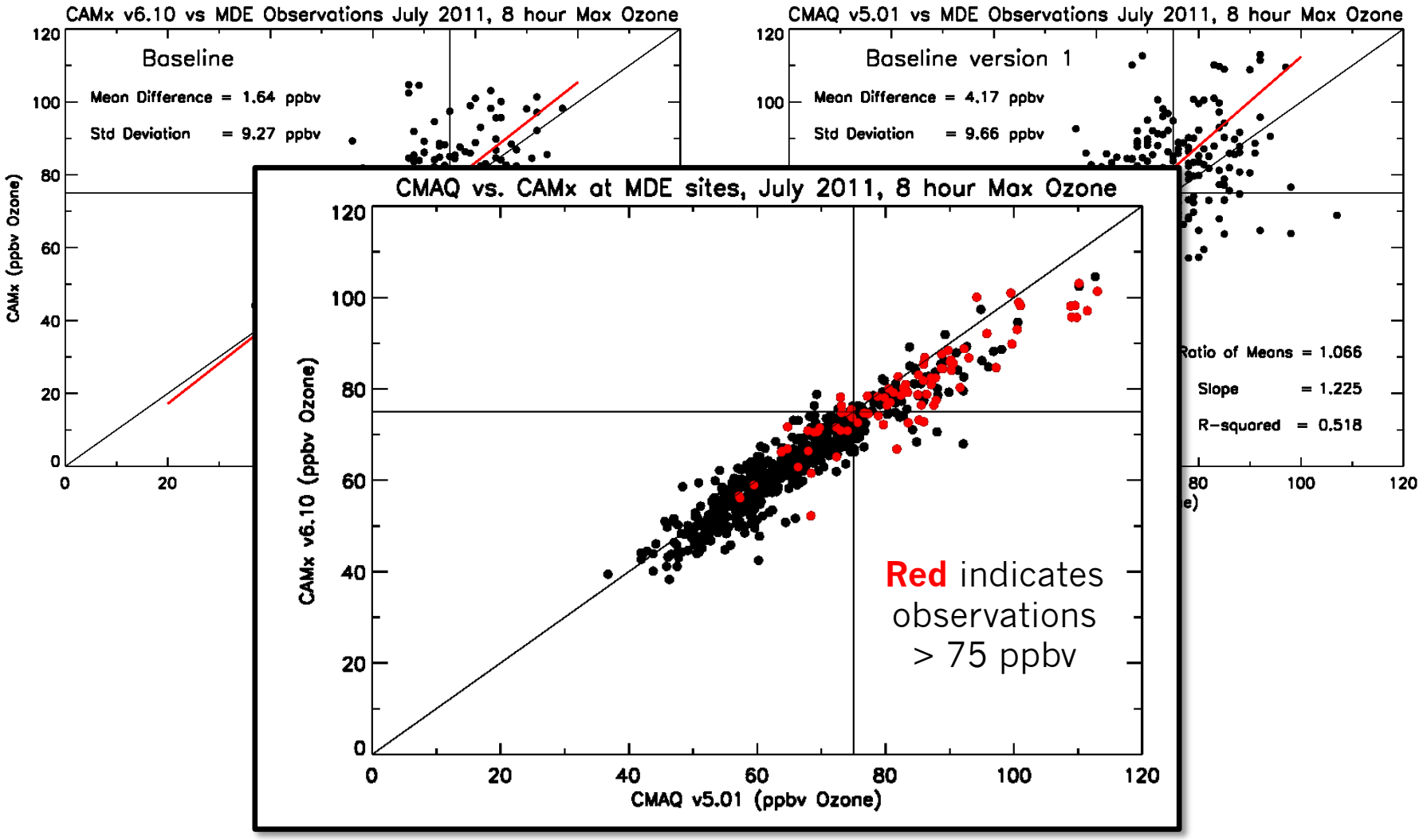
Models compared to observations





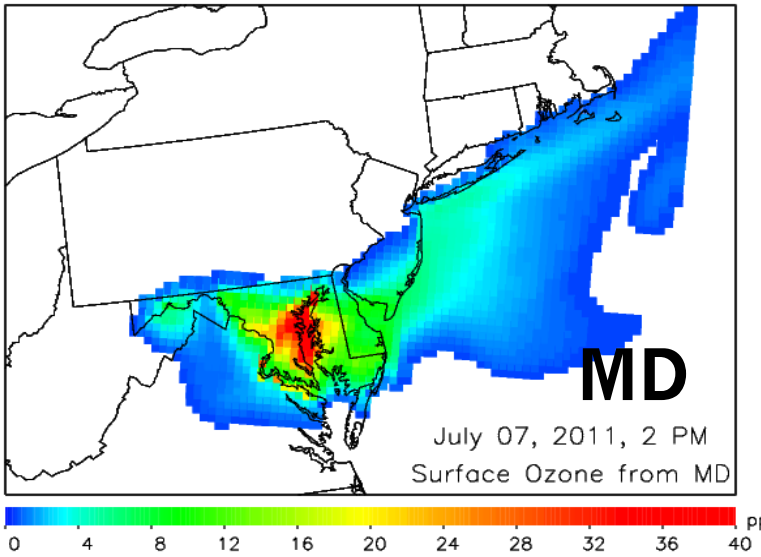
- CAMx performs slightly better at predicting surface ozone using version 1 of the emissions
- CMAQ does better when using model version 5.02 and version 2 alpha of the emissions

Comparison: CAMx vs. CMAQ

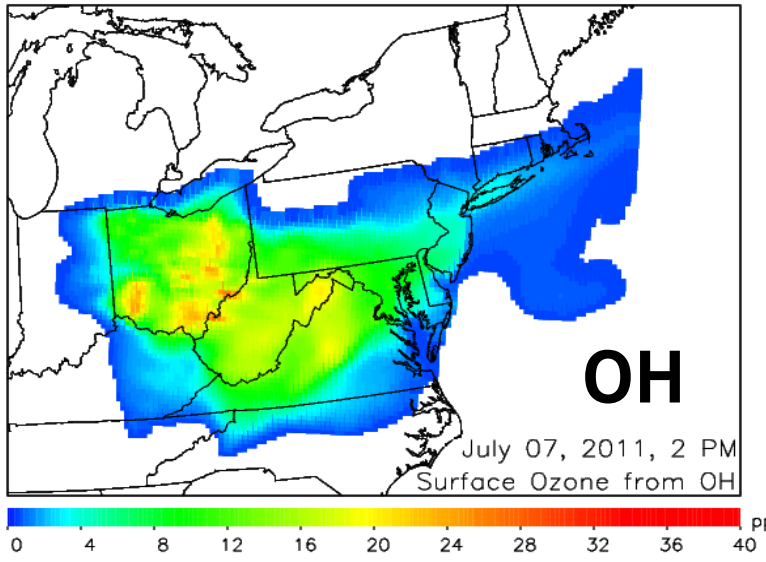


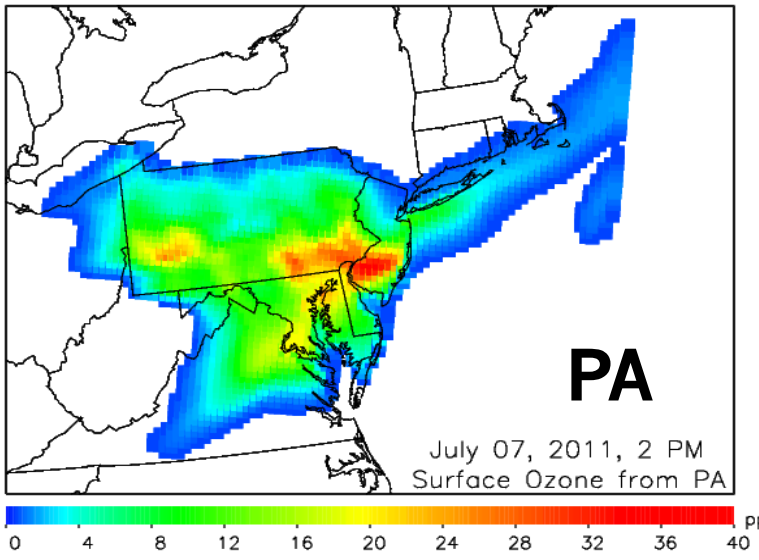
Ozone Source Apportionment

Ozone Source Apportionment Examples



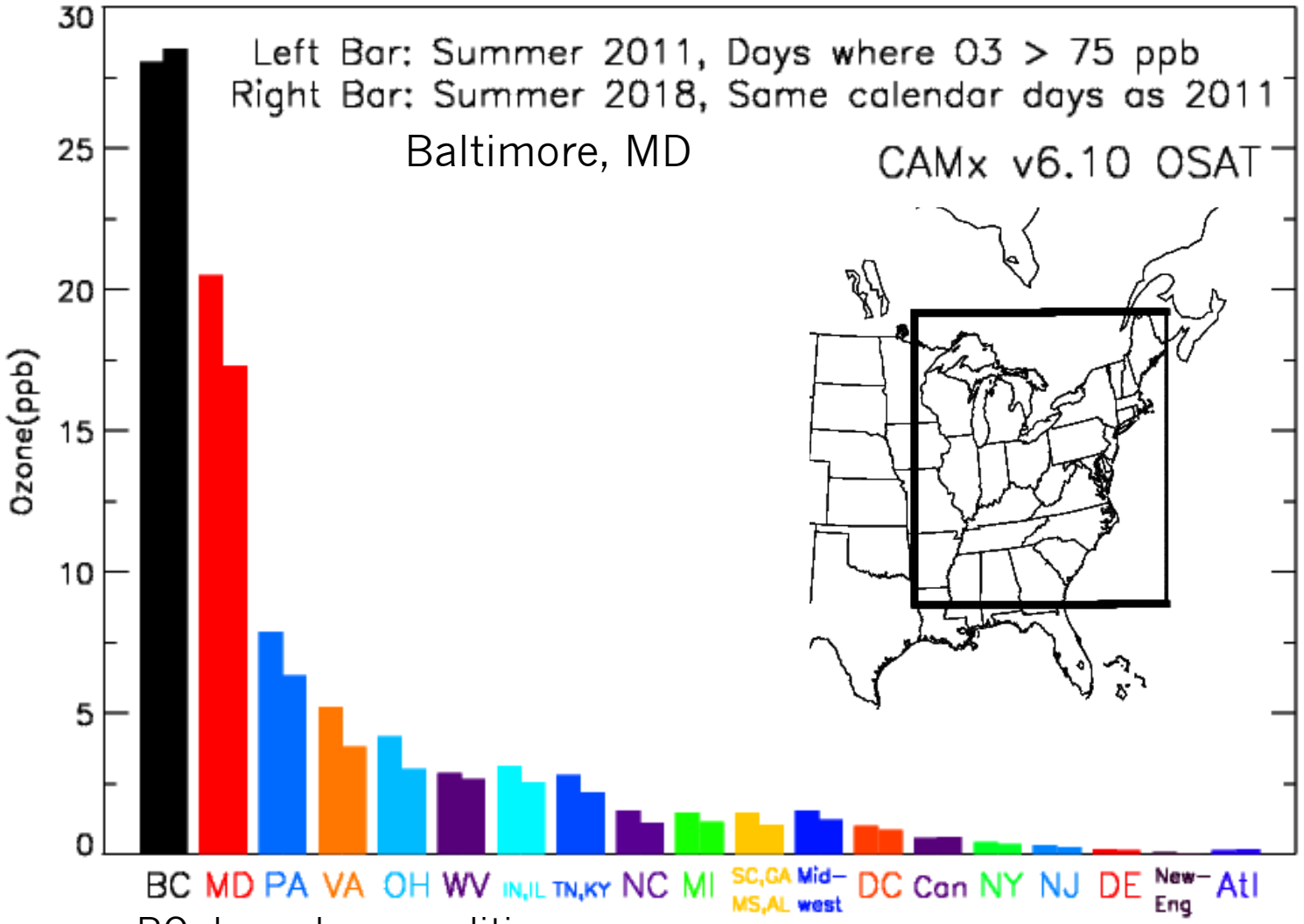
- The CAMx software can attribute ozone to different source regions
- Ozone can be transported long distances downwind of the original source



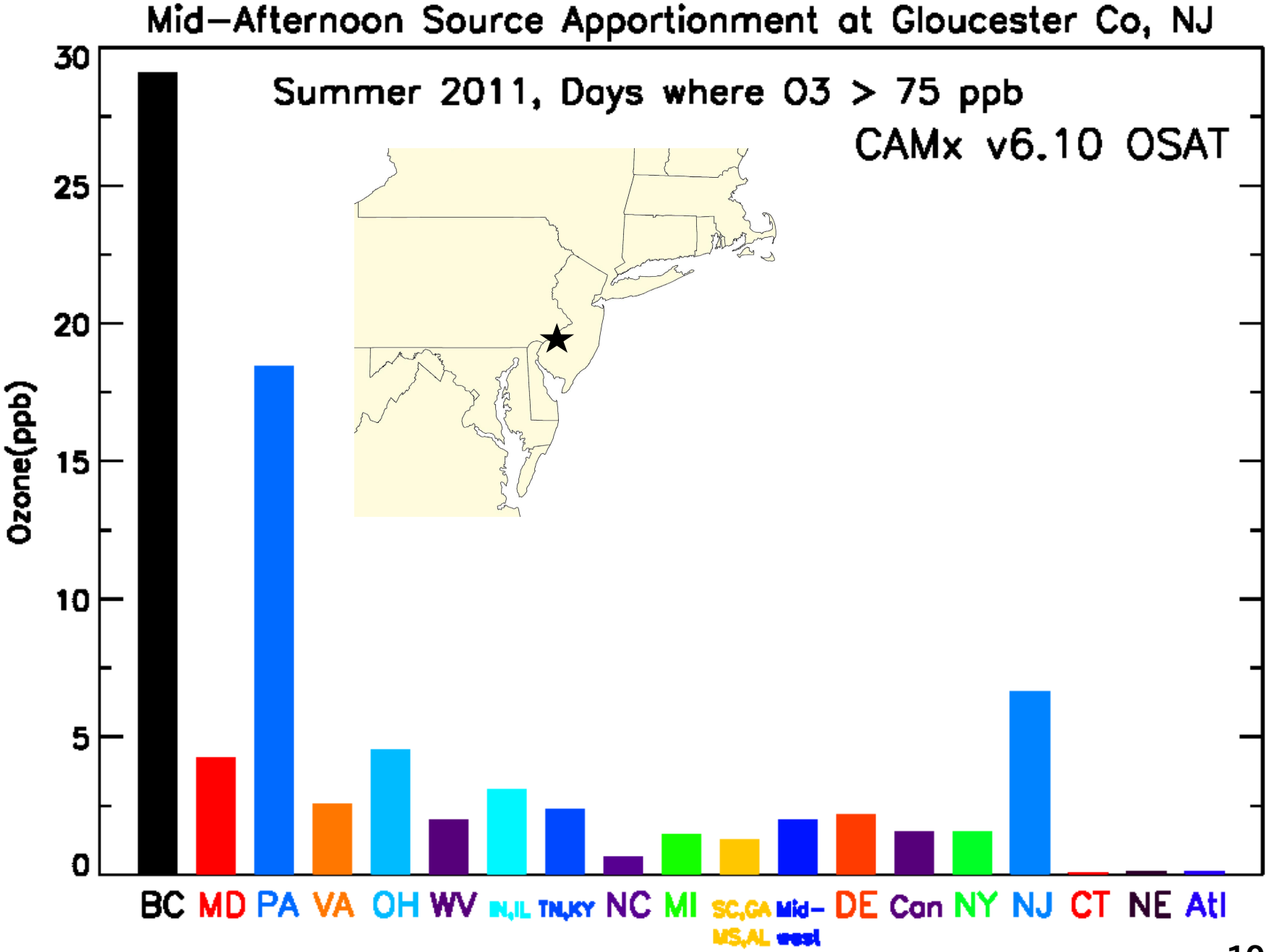


Summer 2011 & 2018: Ozone Source Attribution

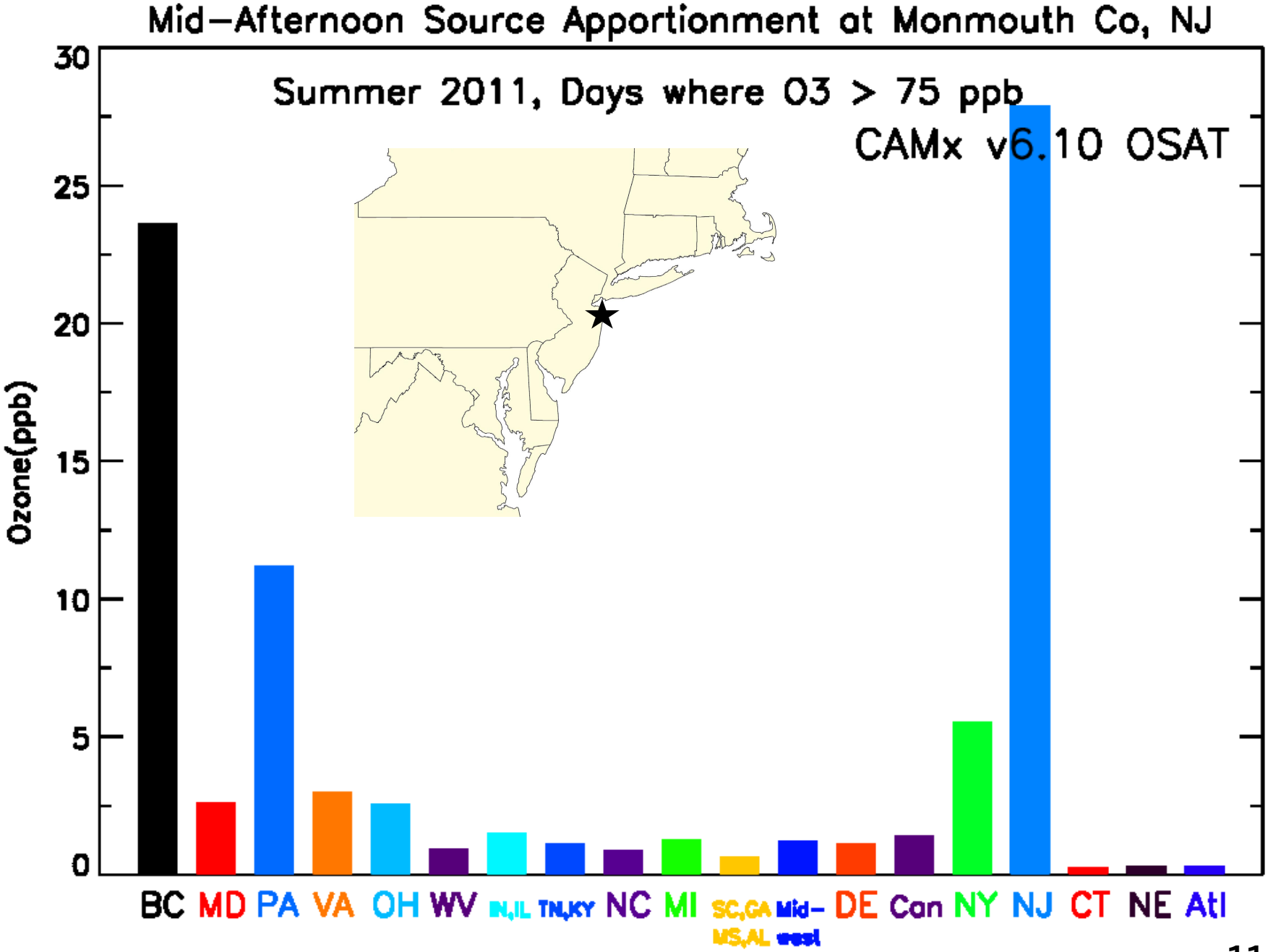
- The attribution of ozone in all states decreases 10 – 25 % over 7 years.
- The only portion to increase is the ozone attributed to the model boundary.



BC=boundary conditions



Preliminary work by Dan Goldberg, University of Maryland, please contact prior to use



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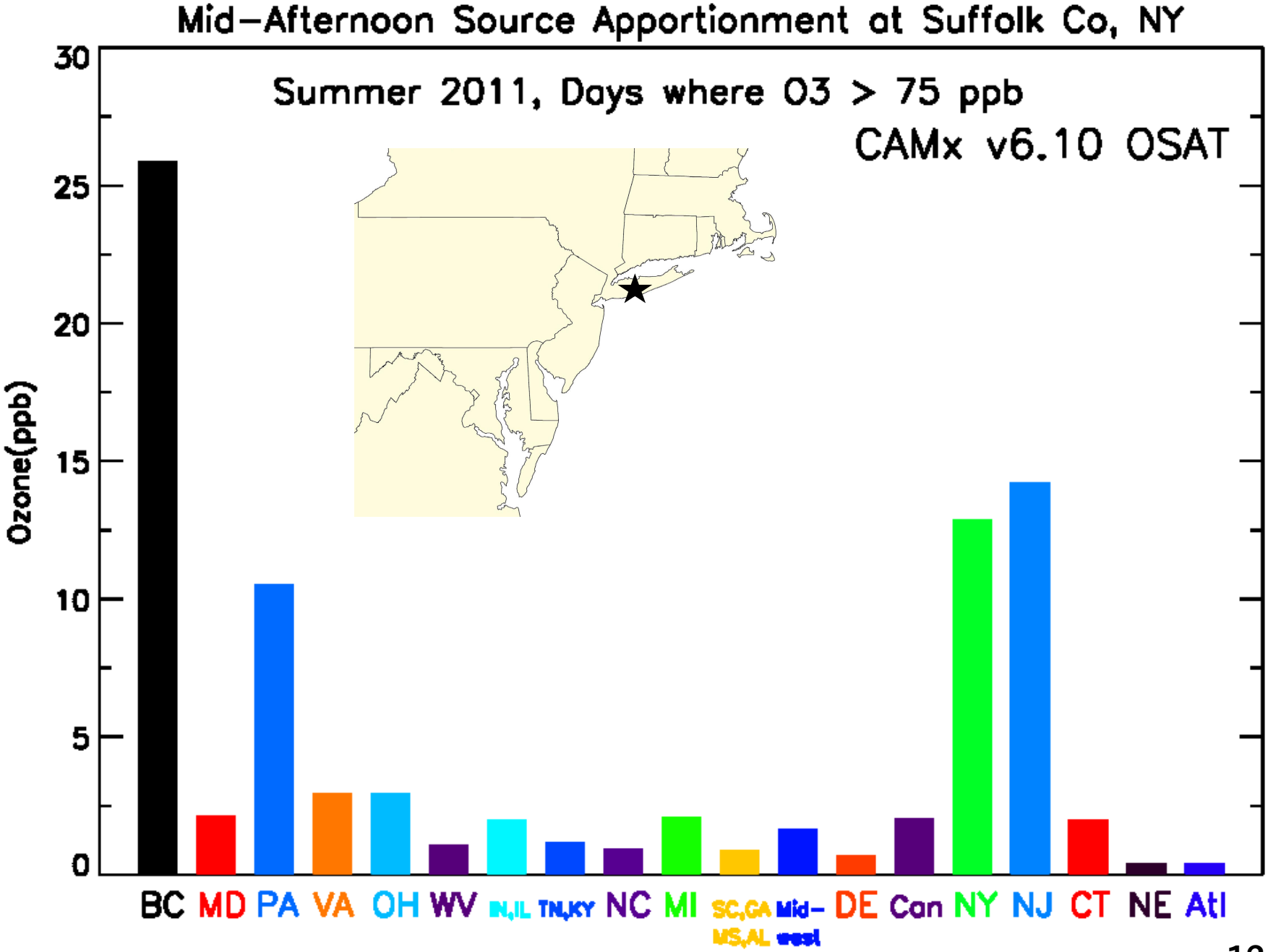

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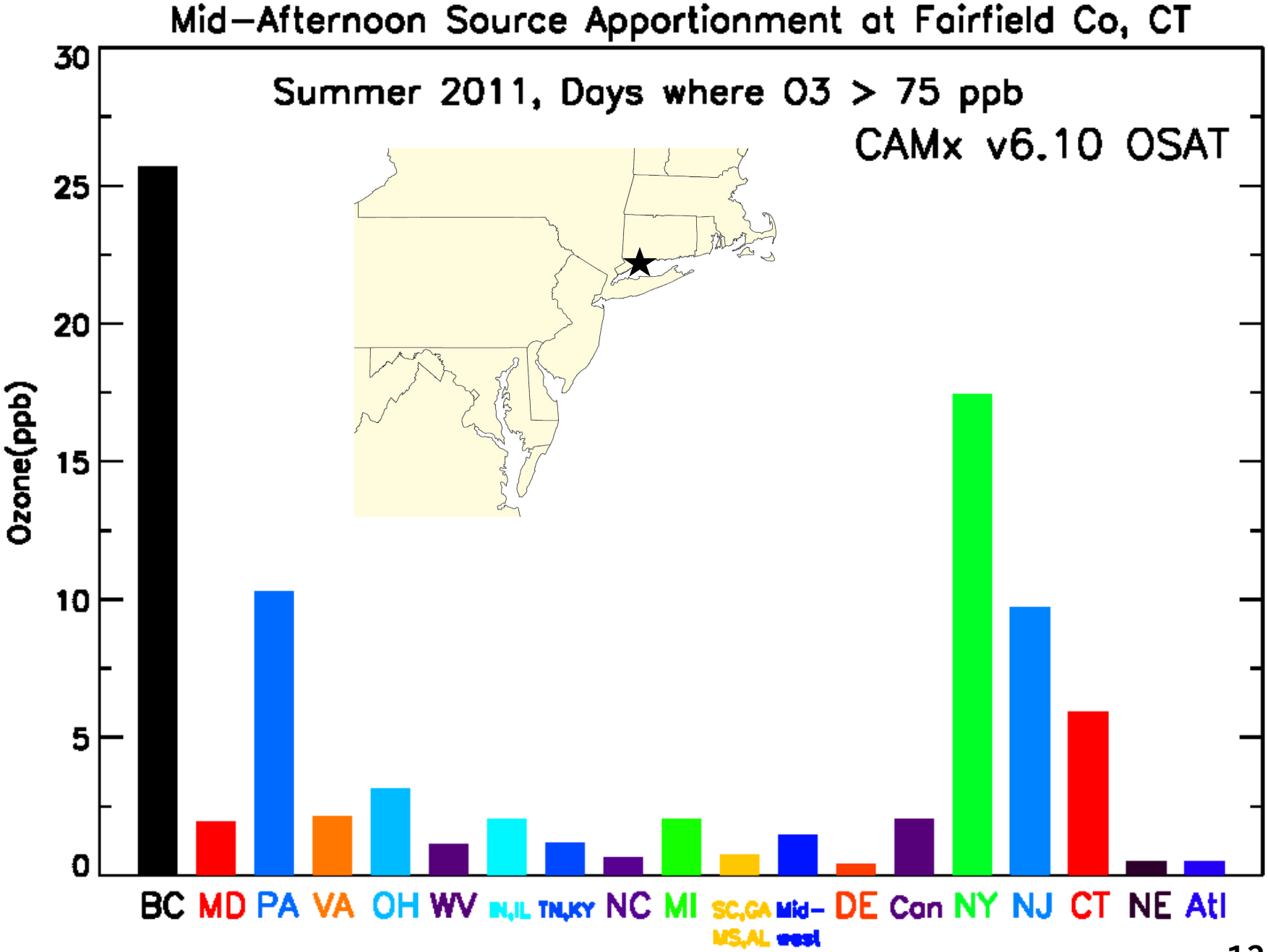

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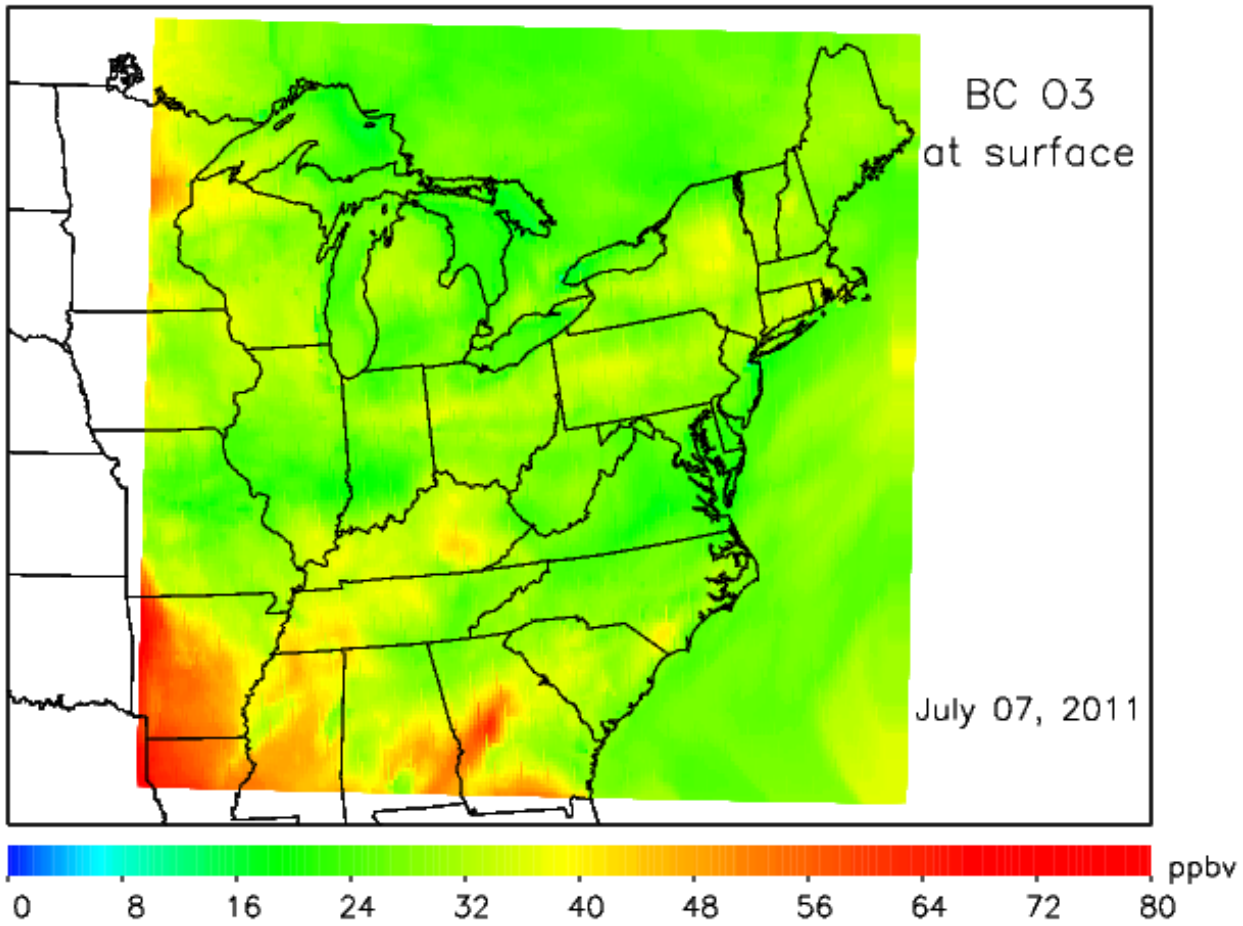
Boundary Ozone

Ozone from the model boundary

Ozone attributed to areas beyond the model domain, i.e., Texas, Cal, Asia



- Ozone from the boundary is uniformly greater than 15 ppbv.
- Some locations, especially close to the boundaries, are higher.

July 2011: Ozone attributed to the Model Domain Boundaries

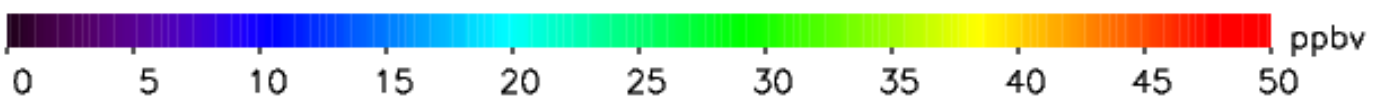
~2/3rds of Boundary ozone in Maryland came from the Western Boundary

West

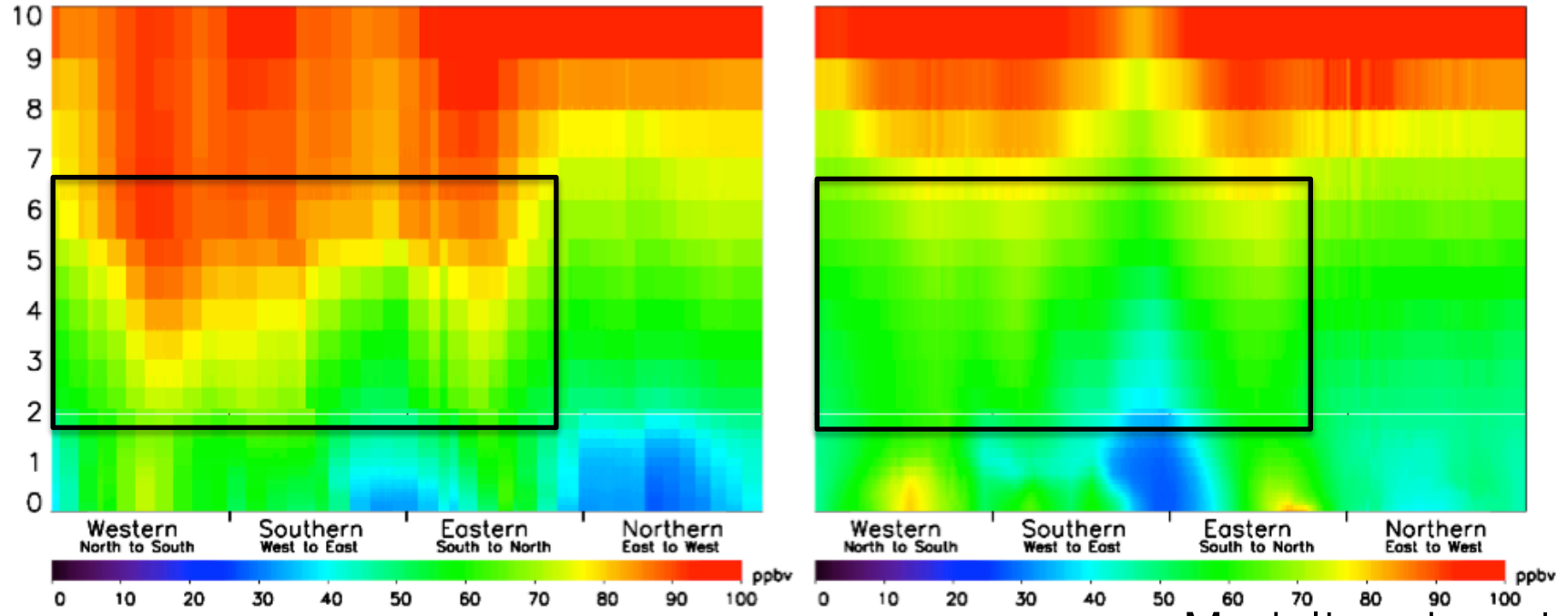
East

South

North



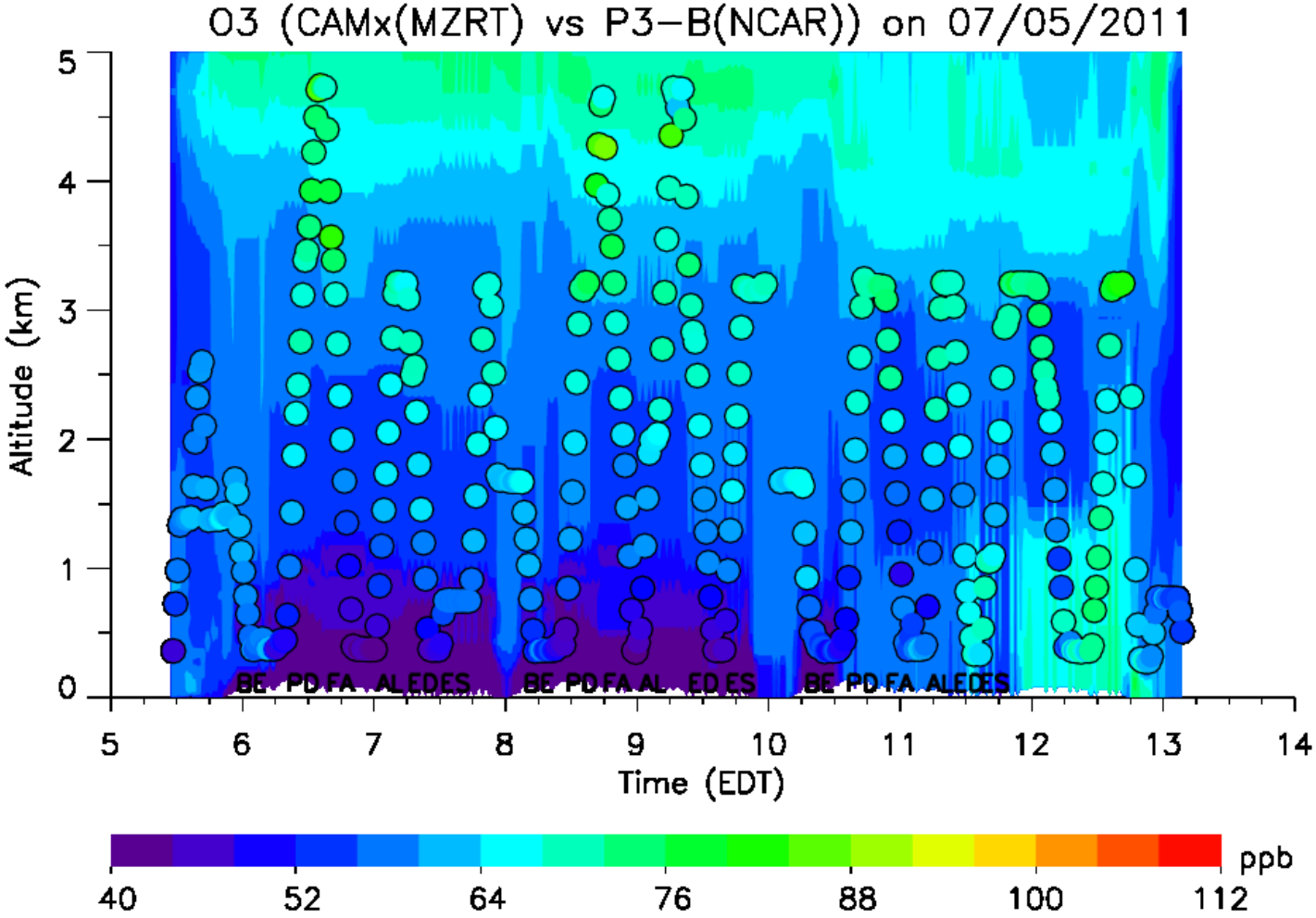
Curtain plots of Ozone at the Boundary during July 2011



Modeling domain

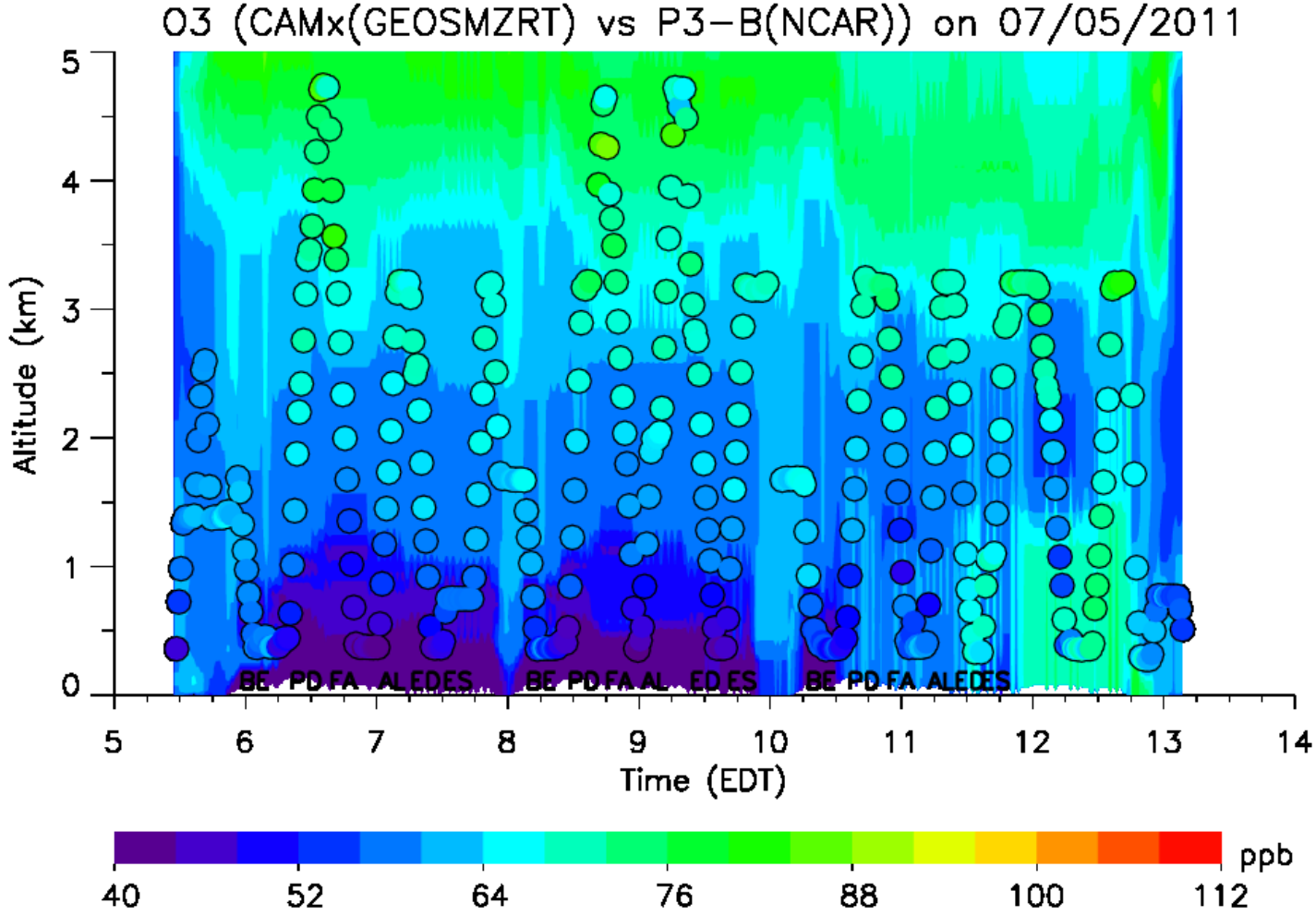
- MOZART is marginally higher in the lower layers at all boundaries, except the Southeast.
- GEOS–Chem has higher ozone in the mid–troposphere, *especially at the western boundary* (which is the boundary that most often influences ozone in the eastern United States).

Sensitivity study: **MOZART** vs. GEOS-Chem Boundary Conditions



Ozone aloft is poorly represented in the model

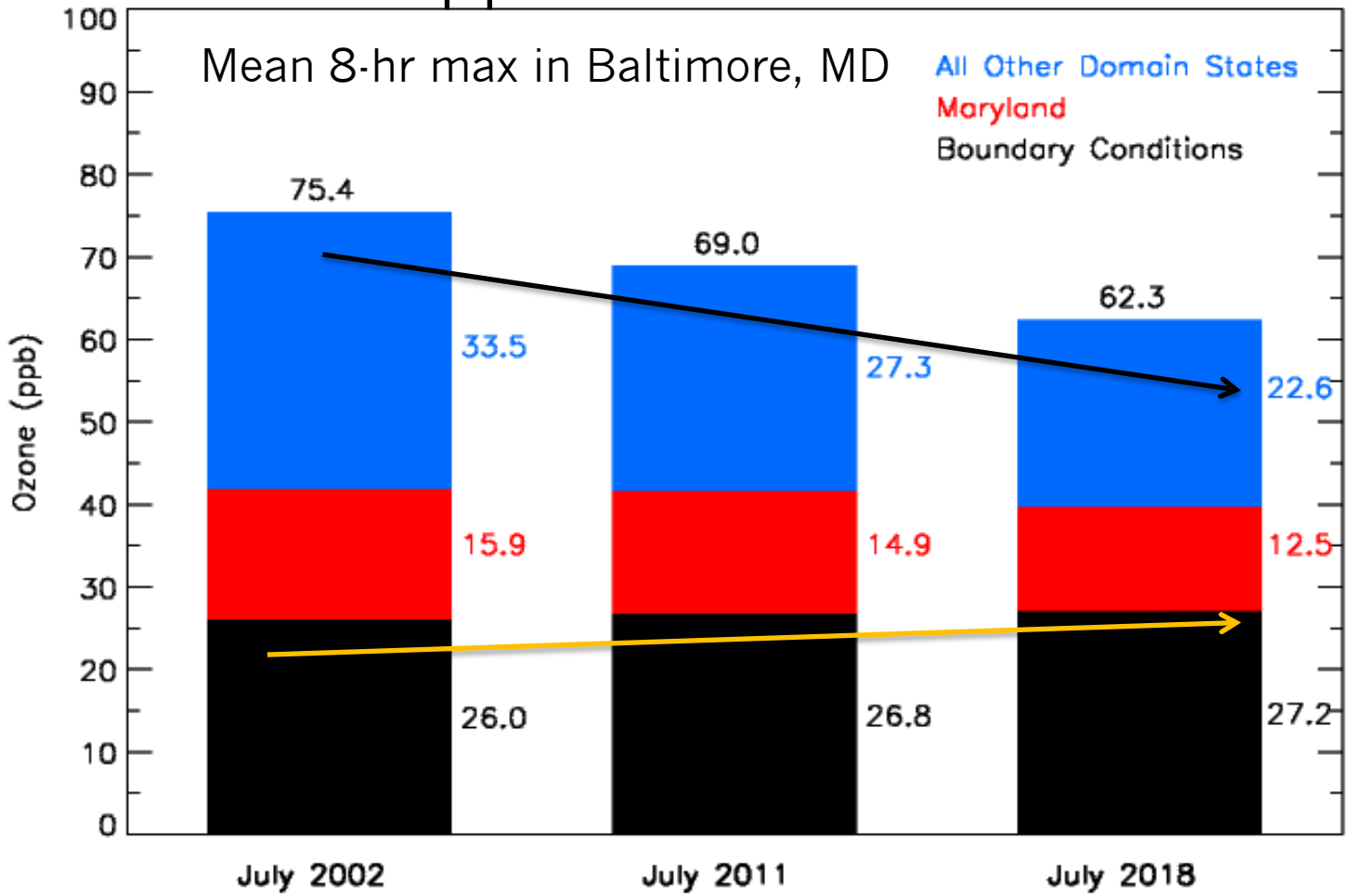
Sensitivity study: MOZART vs. **GEOS-Chem** Boundary Conditions



More ozone aloft when using GEOS-Chem, which better agrees with observations!
… but still underestimated especially between 1 – 3 km agl

Evidence for an Increase in the Photochemical Lifetime of Ozone

Trends in the Apportionment of Surface Ozone



- Boundary and meteorology are initialized *identically* in each simulation.
- Total surface ozone has decreased and is projected to further decrease.
  - Sources inside the model domain will decrease.
  - **If the sources outside the model domain remain the same, ozone attributed to these sources will increase.**

Goldberg et al., Submitted, *JGR*

Trends in the Apportionment of Surface Ozone

Mean July percentage of ozone (%) attributed to the boundary

Metropolitan Area	2002	2011	2018
New York, NY	37.0%	41.6%	45.3%
Philadelphia, PA	38.1%	42.7%	47.6%
Baltimore, MD	34.5%	38.8%	43.6%
Washington, DC	35.9%	41.0%	46.5%

Mean July concentration of ozone (ppbv) attributed to the boundary

Metropolitan Area	2002	2011	2018
New York, NY	23.9	24.6	25.9
Philadelphia, PA	26.8	27.4	27.7
Baltimore, MD	26.0	26.8	27.2
Washington, DC	27.1	27.6	28.0

- An increasing role of the boundary is seen in all metropolitan areas in the eastern United States.

Goldberg et al., Submitted, *JGR*

Trends in the Apportionment of Surface Ozone

Mean July percentage of ozone (%) attributed to the boundary

What is causing this increase???

Ironically, we think it's related to reductions in NO_x and VOCs

Reductions in NO_x and VOCs are causing the ozone lifetime to increase!

*See supplementary material for more detail

Mean J … oundary

Philadelphia, PA	26.8	27.4	27.7
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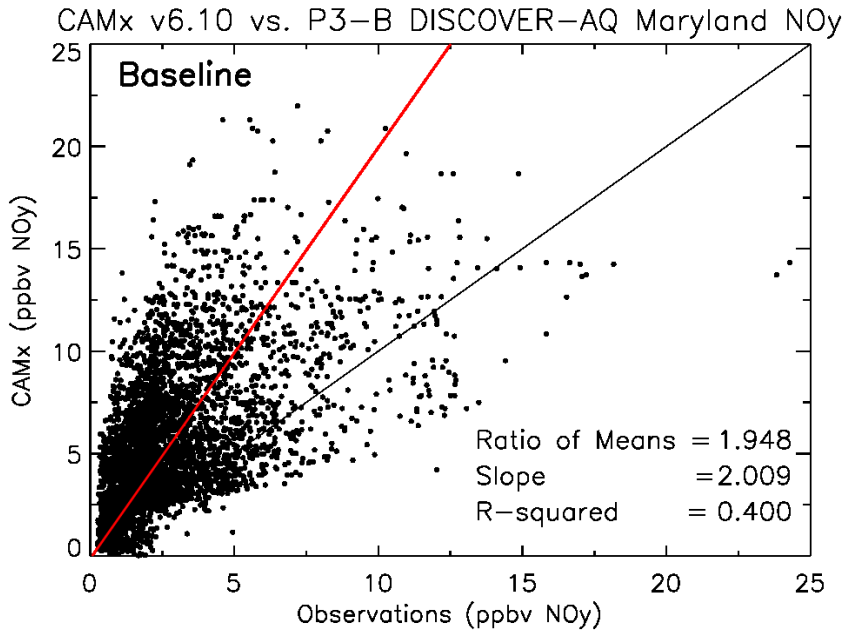
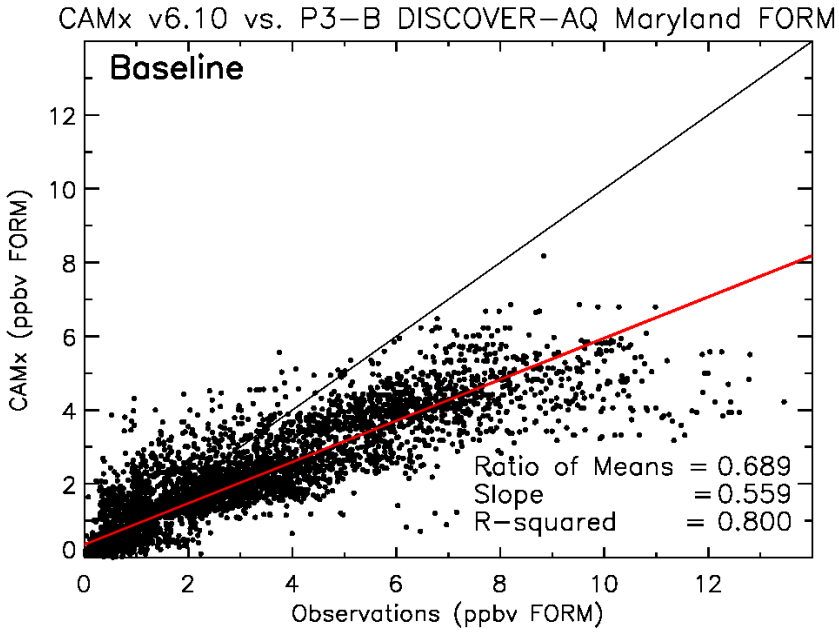
Updates to the Modeling Platform that better predict Ozone Precursors

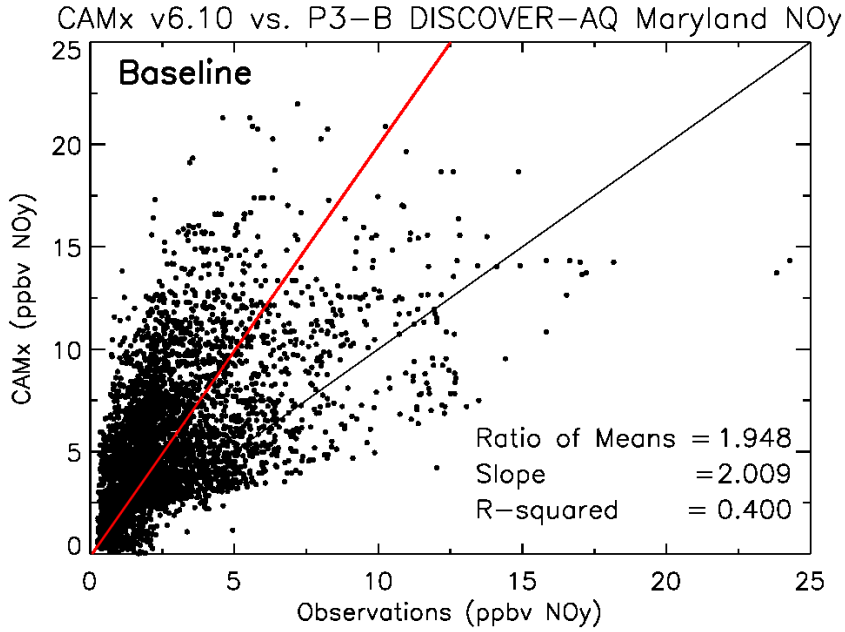
Prediction of O_3 precursors: Using DISCOVER-AQ data

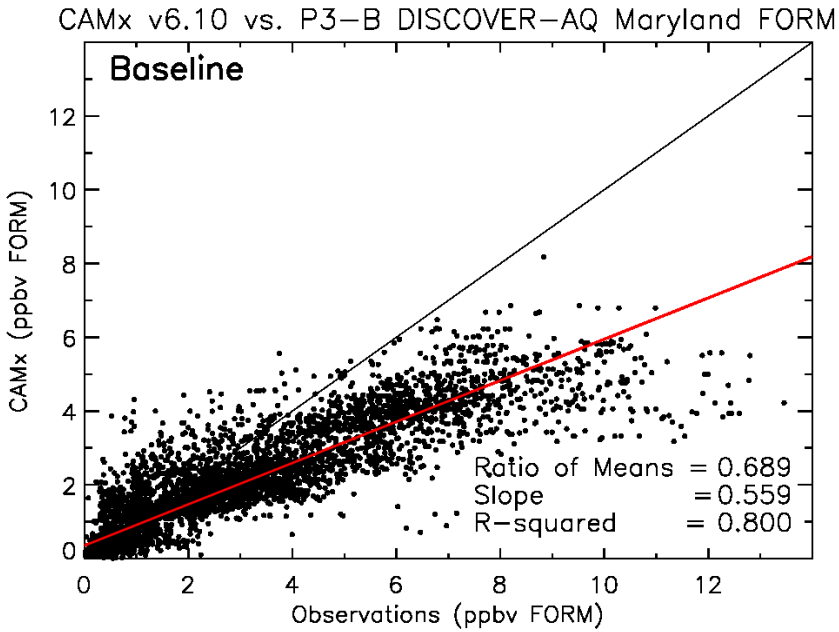




- The comparison with data from the P3-B aircraft during DISCOVER-AQ MD shows a significant over prediction of NO_y and a significant under prediction of HCHO.

Prediction of O_3 precursors: Using DISCOVER-AQ data

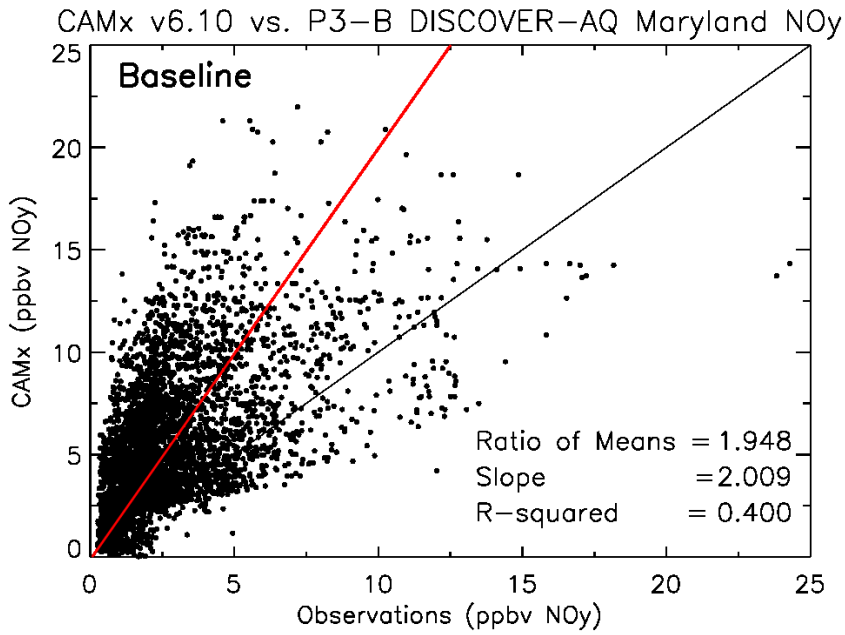


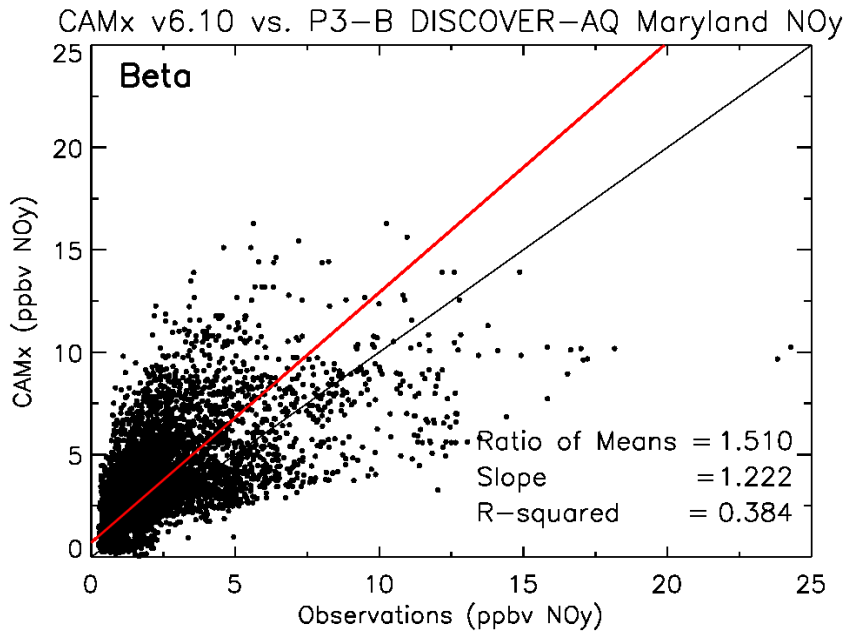


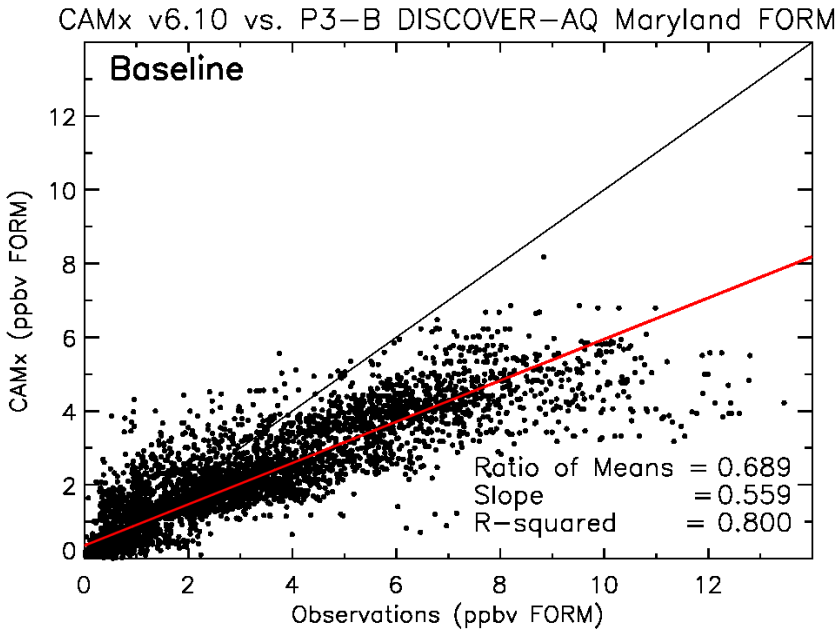
- The comparison with data from the P3-B aircraft during DISCOVER-AQ MD shows a significant over prediction of NO_y and a significant under prediction of HCHO.

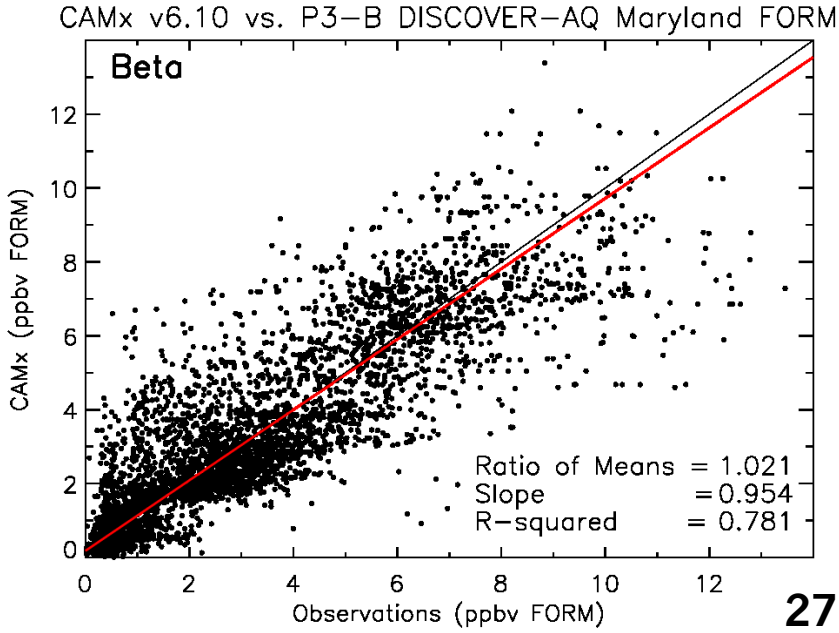
- We've made three changes to update the model, "Beta":
  - CB6r2 gas-phase chemistry (Old: CB05)
  - MEGAN v2.1 biogenic emissions (Old: BEISv3.14)
  - Reduce emissions from mobile sources by 50% (Anderson et al., 2014)

Prediction of O_3 precursors: Using DISCOVER-AQ data

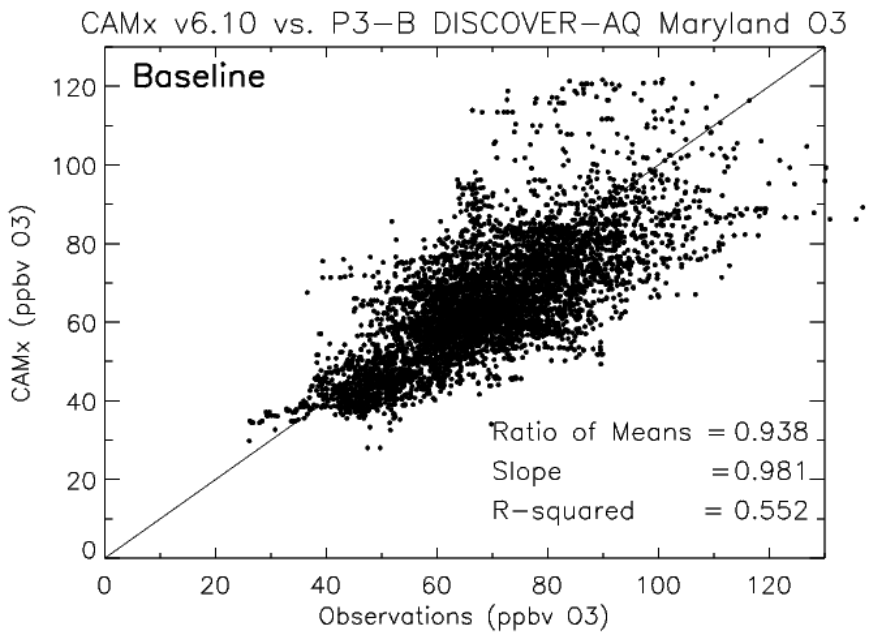


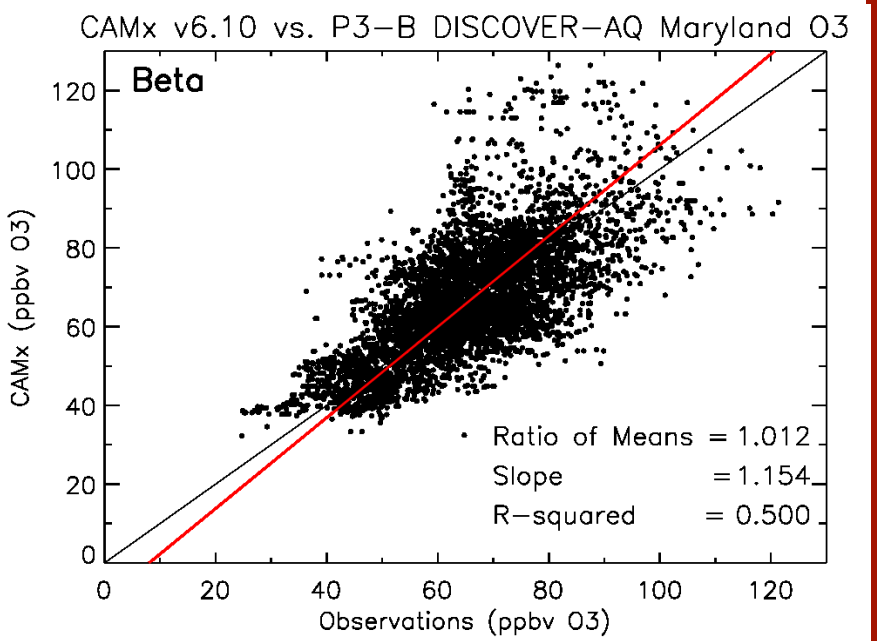






Prediction of O_3: Using DISCOVER-AQ data





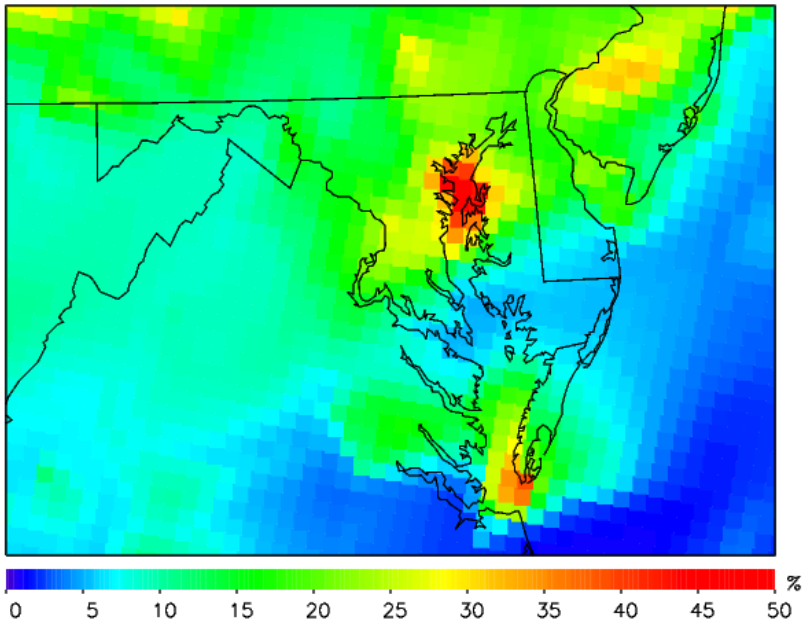
- Prediction of ozone is similar in each case, but *how* the ozone produced is much different

*Using the updated O3 data adjusted for the water vapor interference (this data is not in the D-AQ data archive).

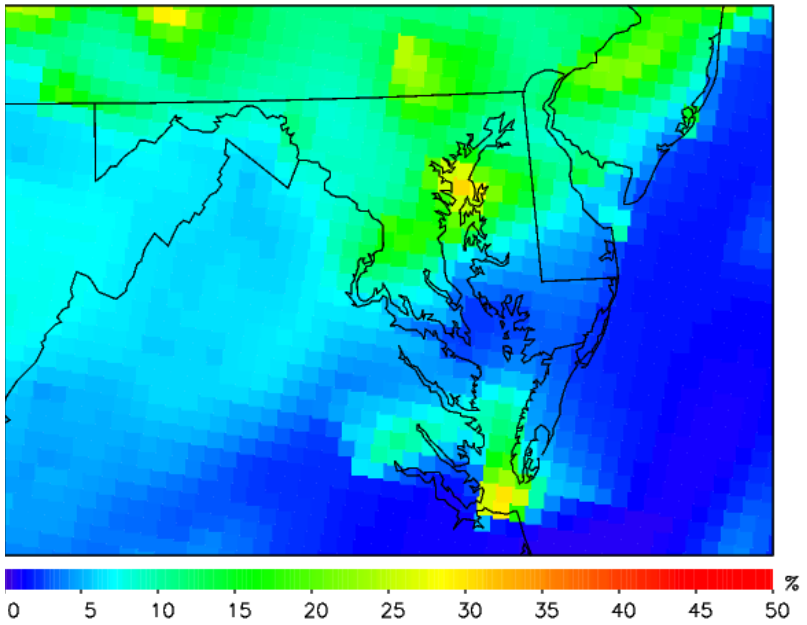
Policy Implications of the model updates

Percentage of O_3 formed in a VOC-limited environment during the daytime of July 7, 2011

Baseline



Beta

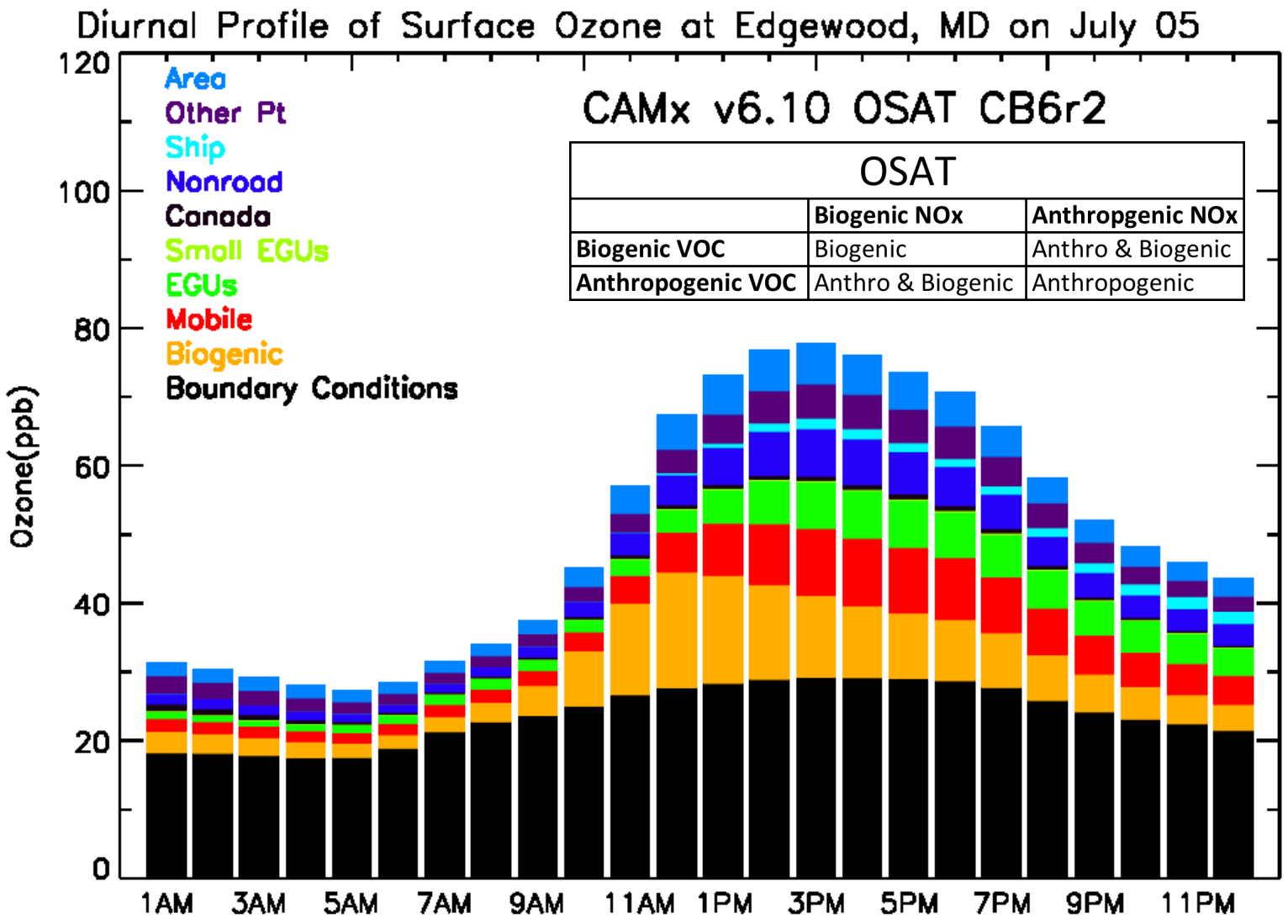


- The model will be more responsive to NO_x emission changes.

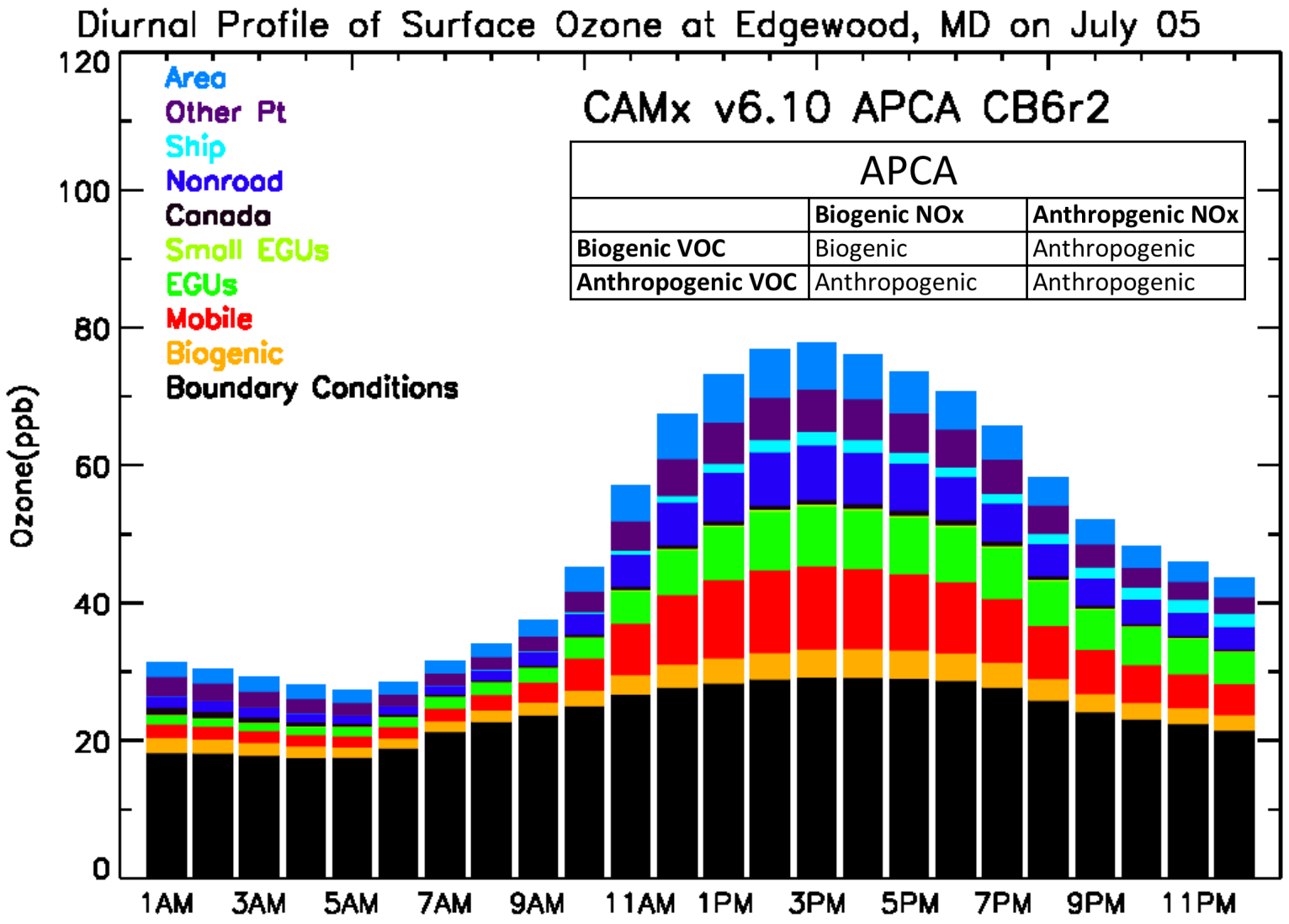
Application of Source Apportionment Modeling OSAT and APCA

*OSAT= Ozone Source Apportionment Tool
*APCA=Anthropogenic Precursor Culpability Assessment

Example: OSAT vs. APCA: OSAT

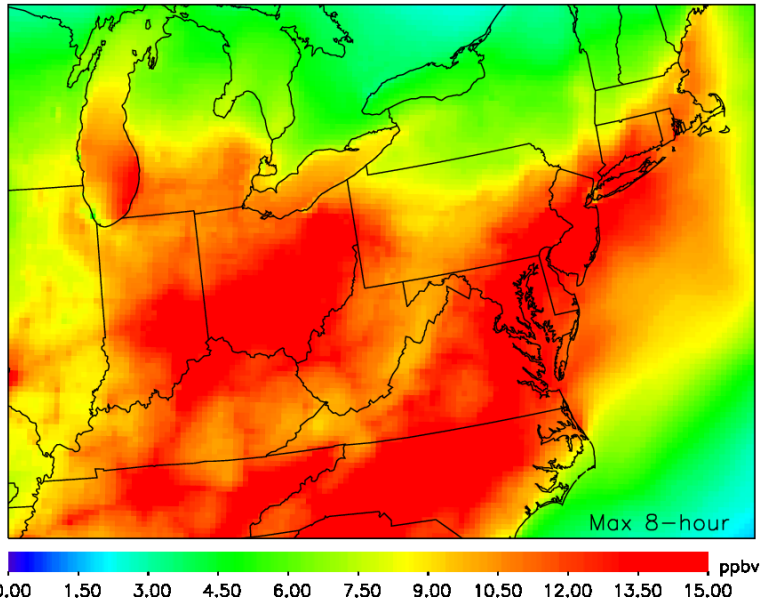


Example: OSAT vs. APCA: APCA

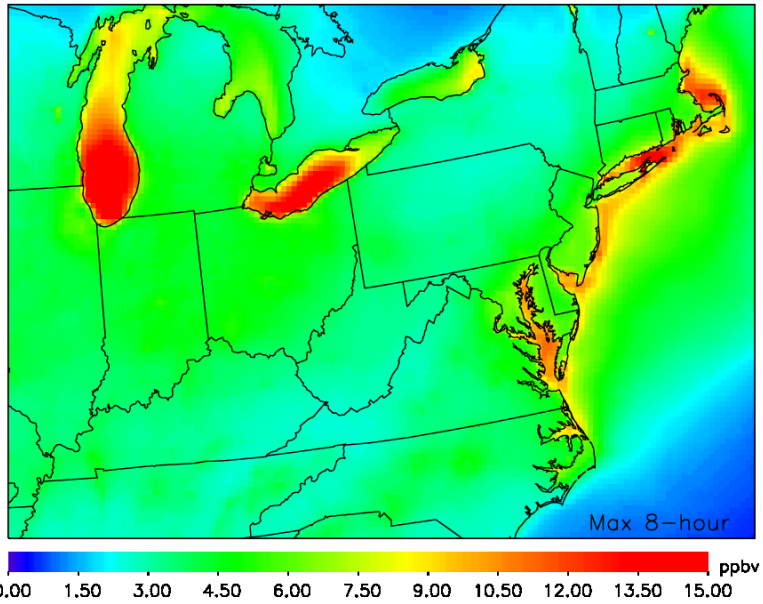


2011 APCA: Version 2 Emissions

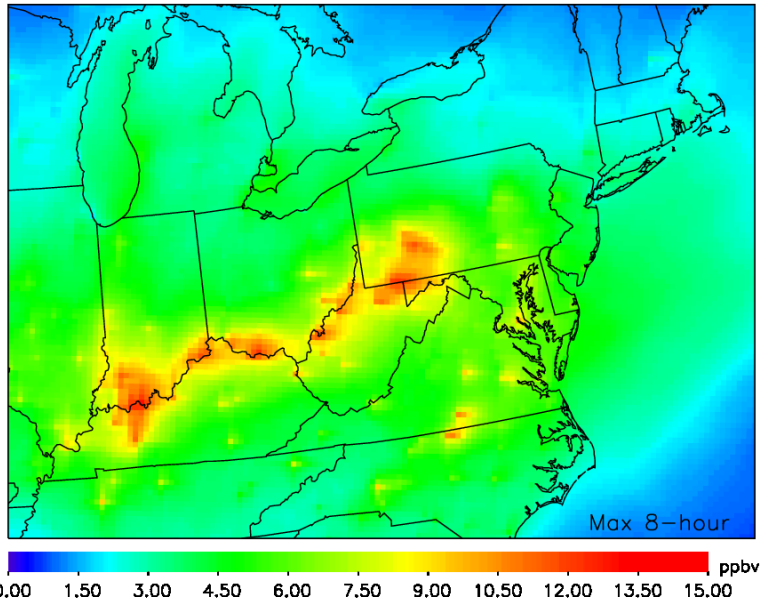
July 2011 Mean Surface O3 from On– & Off–road



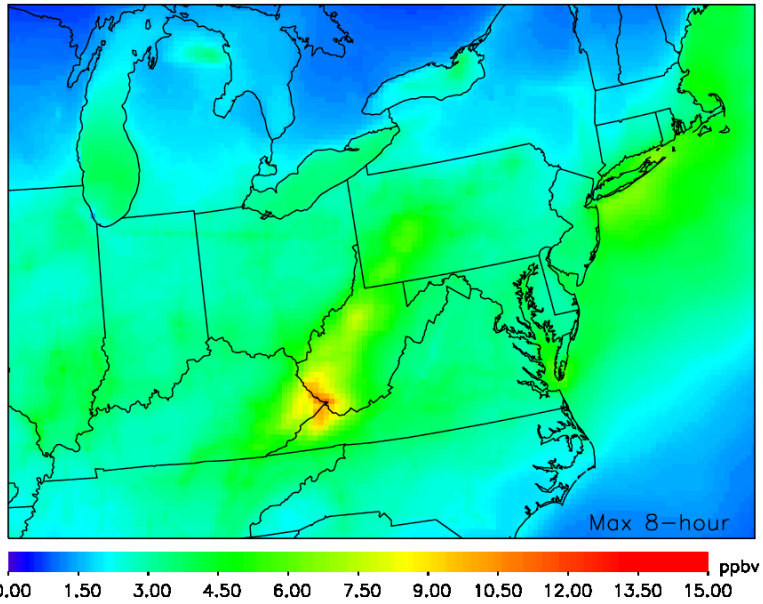
July 2011 Mean Surface O3 from Nonroad



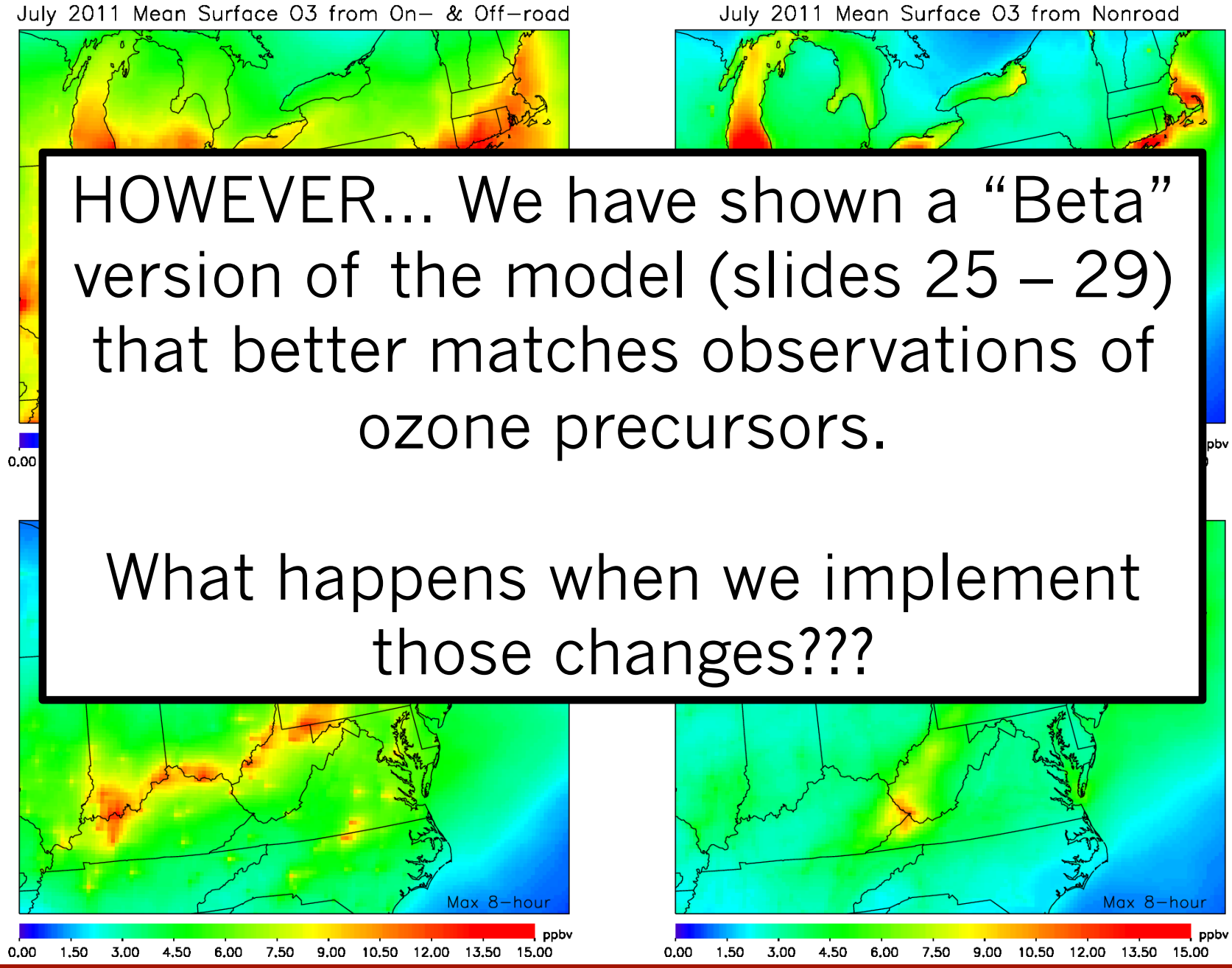
July 2011 Mean Surface O3 from EGUs



July 2011 Mean Surface O3 from Area Sources



2011 APCA: Version 2 Emissions

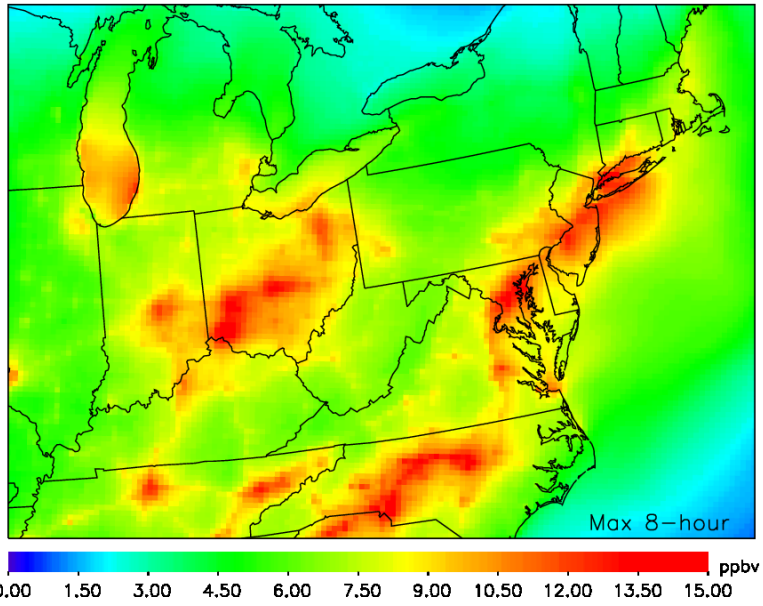


HOWEVER… We have shown a "Beta" version of the model (slides 25 – 29) that better matches observations of ozone precursors.

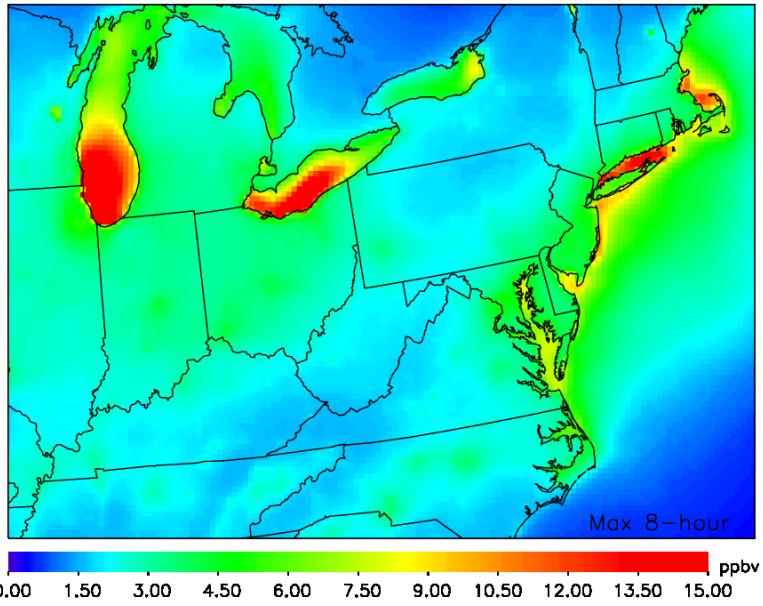
What happens when we implement those changes???

2011 APCA Beta: Version 2 Emissions

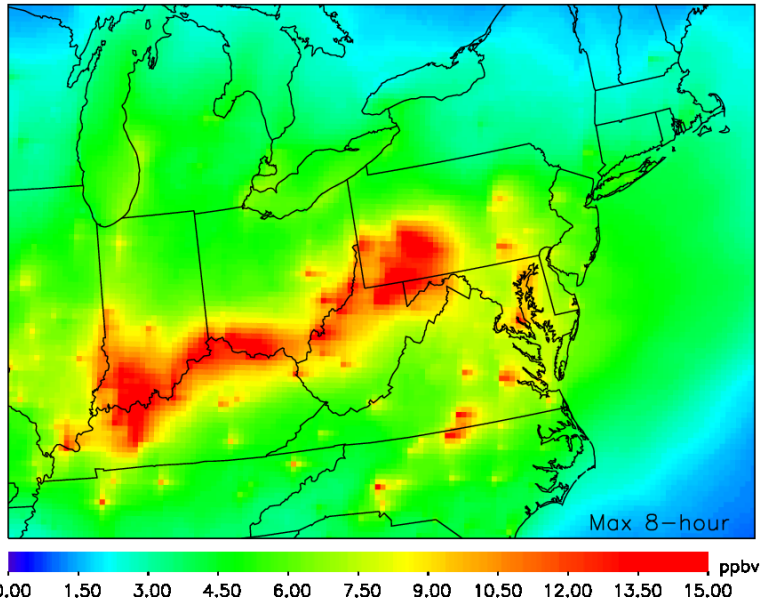
July 2011 Mean Surface O3 from On– & Off–road



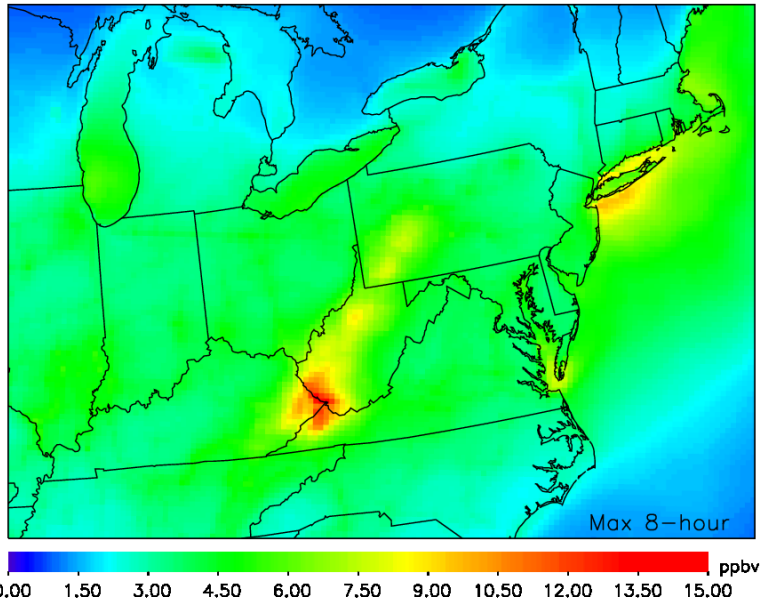
July 2011 Mean Surface O3 from Nonroad



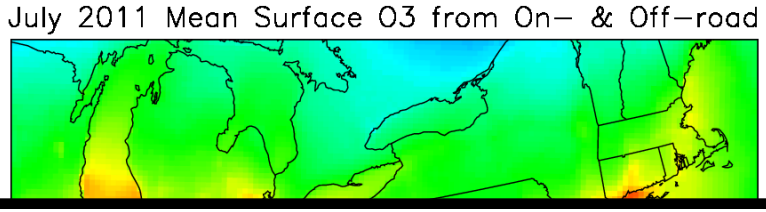
July 2011 Mean Surface O3 from EGUs

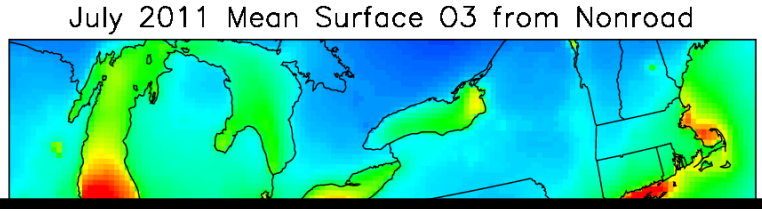


July 2011 Mean Surface O3 from Area Sources

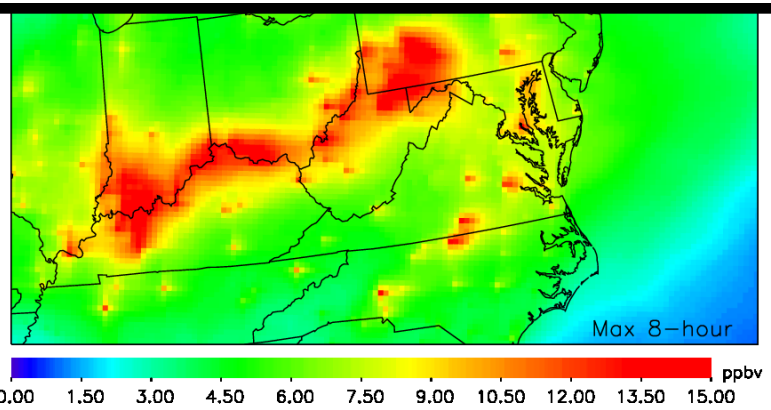


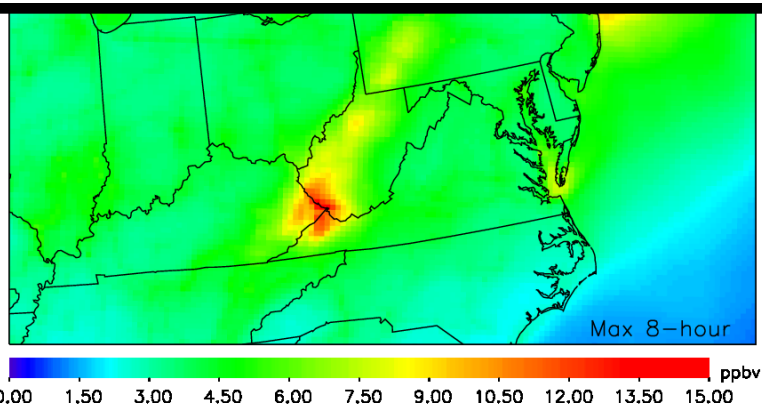
2011 APCA Beta: Version 2 Emissions



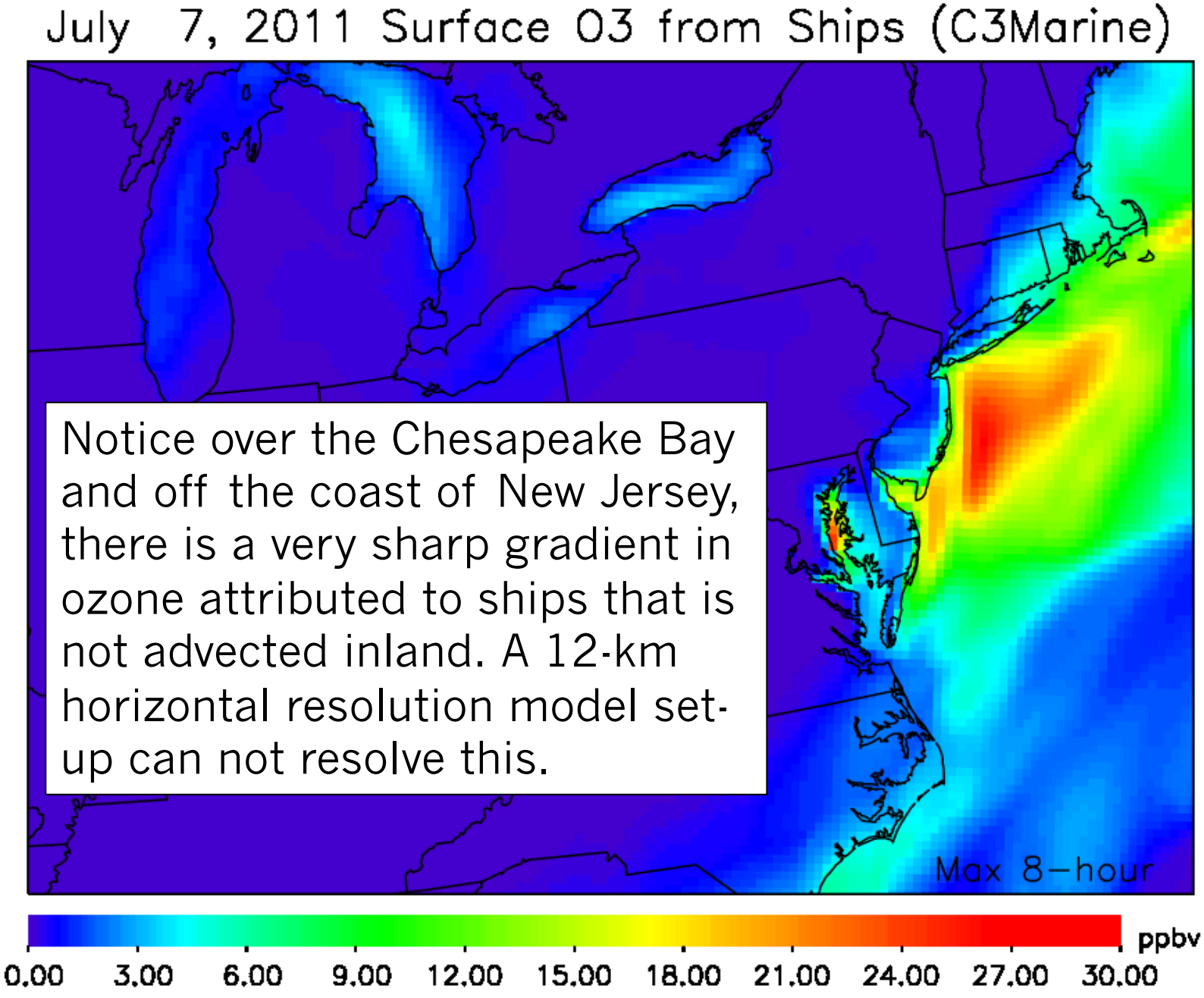


- Ozone attributed to on-road and non-road mobile sources *decreases*
- Ozone attributed to EGUs and area sources *increases*
- In the original simulation, mobile sources dominated the attribution, but now mobile sources and EGUs have the same order of magnitude in Maryland.

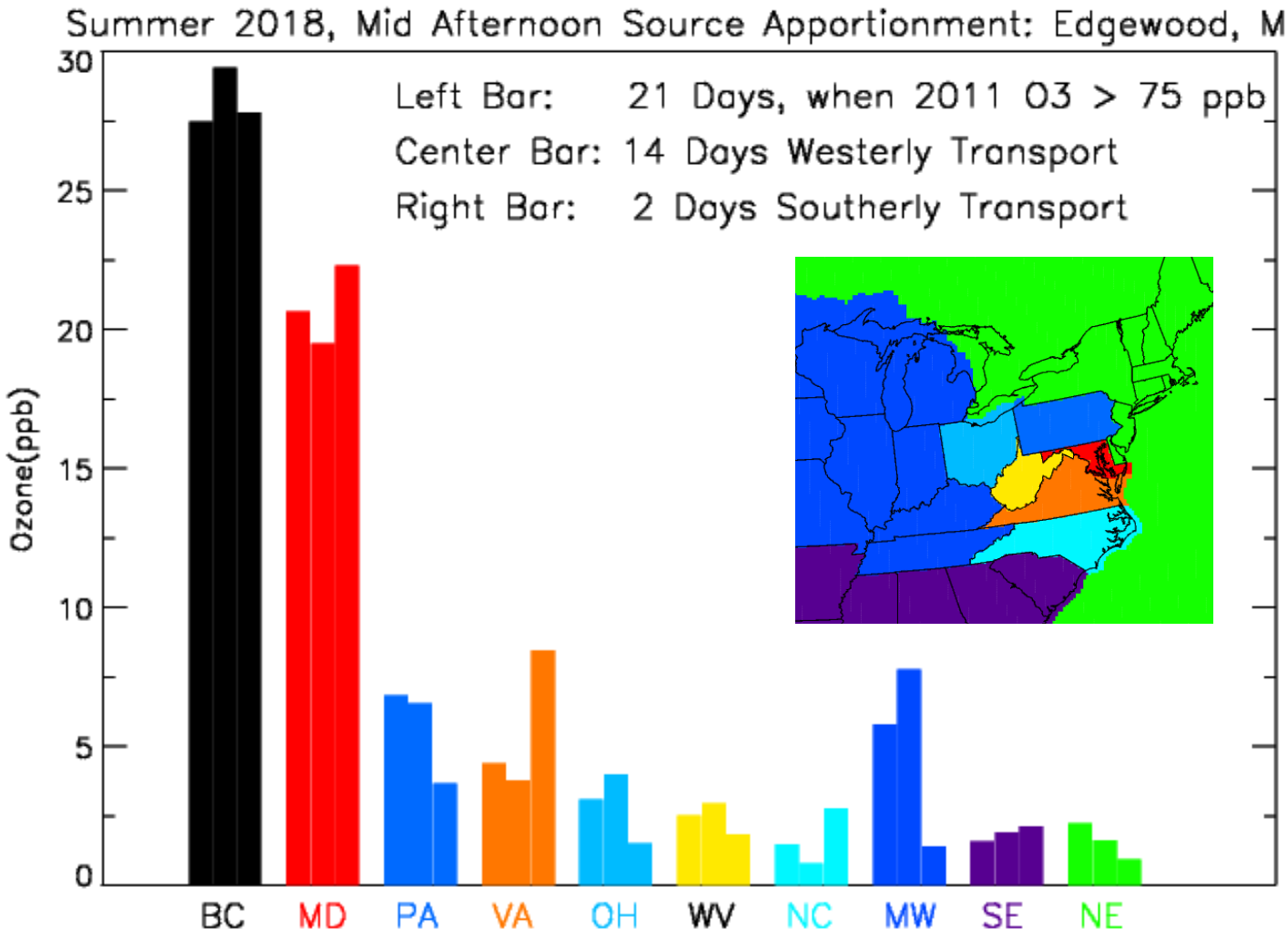




Miscellaneous


July 7, 2011 Surface O3 from Ships (C3Marine)
Notice over the Chesapeake Bay and off the coast of New Jersey, there is a very sharp gradient in ozone attributed to ships that is not advected inland. A 12-km horizontal resolution model set-up can not resolve this.
Max 8-hour
ppbv
0.00
3.00
6.00
9.00
12.00
15.00
18.00
21.00
24.00
27.00
30.00

CAMx OSAT 2018 Source Apportionment by regime type



With help from Joel Dreessen, MDE

- Midwestern & Ohio River valley states have larger role during westerly transport days
- Virginia & North Carolina have double the role during southerly transport days

Conclusions

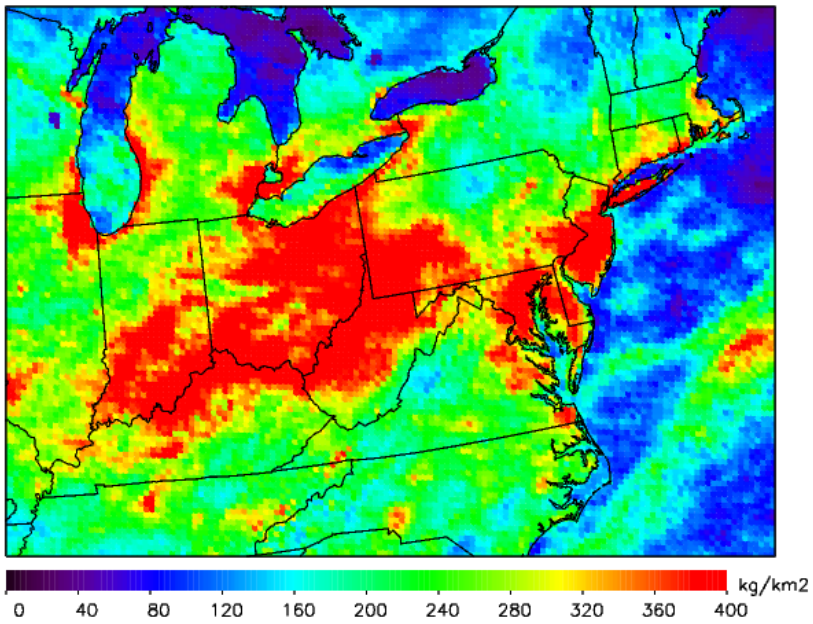
- Baseline version of CAMx shows good agreement with surface ozone observations
- Nonlinearities associated with NO_x and VOC emission reductions are responsible for an increase in the ozone lifetime
  - This is an unintended consequence of the policies to reduce these emissions.
- Updates to the model to give a better prediction of NO_y and HCHO.
  - The model will respond better to reductions in NO_x emissions, which is a better representation of what is happening in reality.

Change in O_3 lifetime due to less NO_x

Assuming 1 mol of O_3 is removed for every 1 mol of HNO_3 deposited.

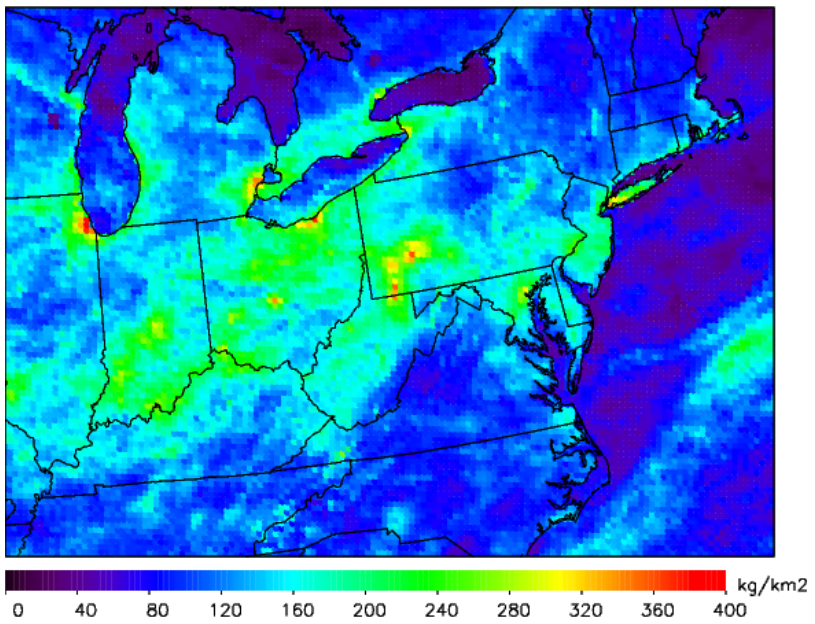
- As HNO_3 deposition decreases, the lifetime of ozone will increase

July 2002



τ_{O3} = 19.2 days

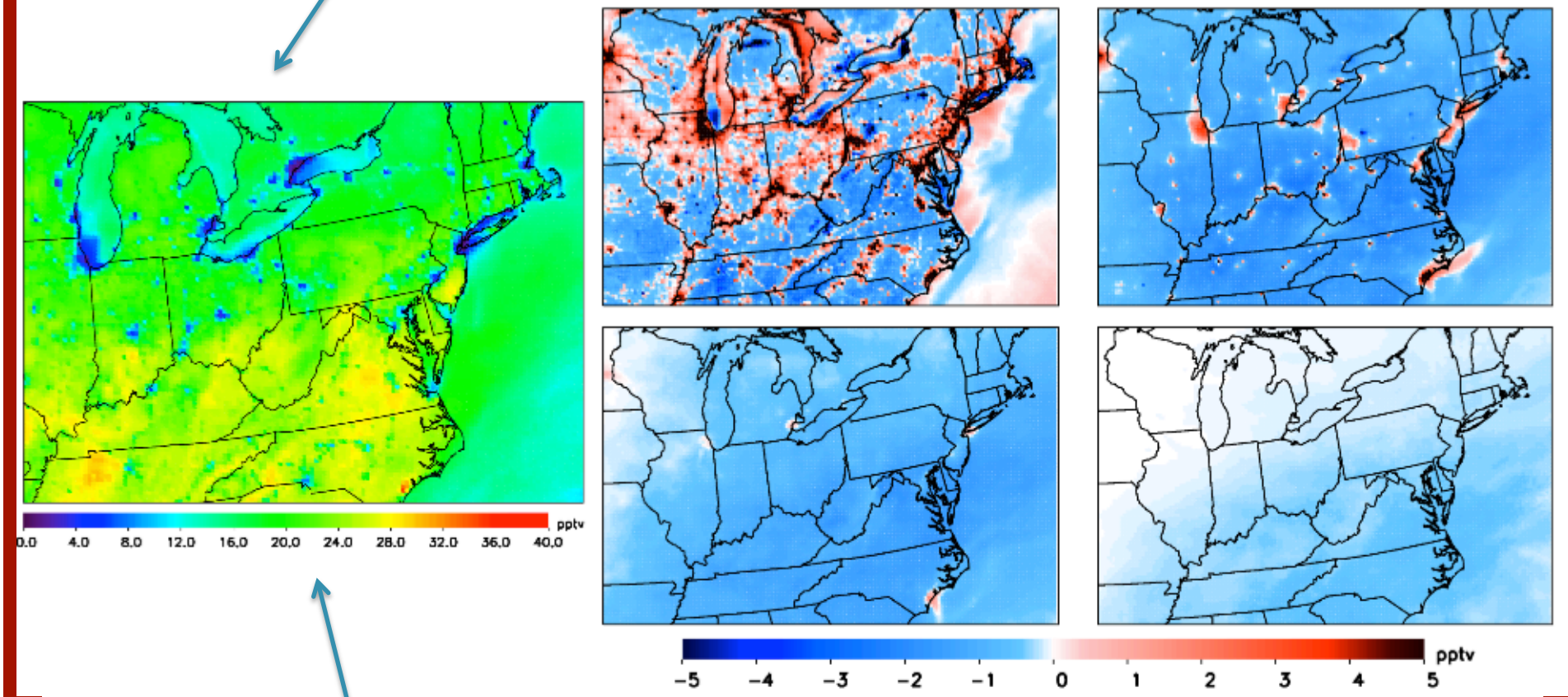
July 2018



τ_{O3} = 28.6 days

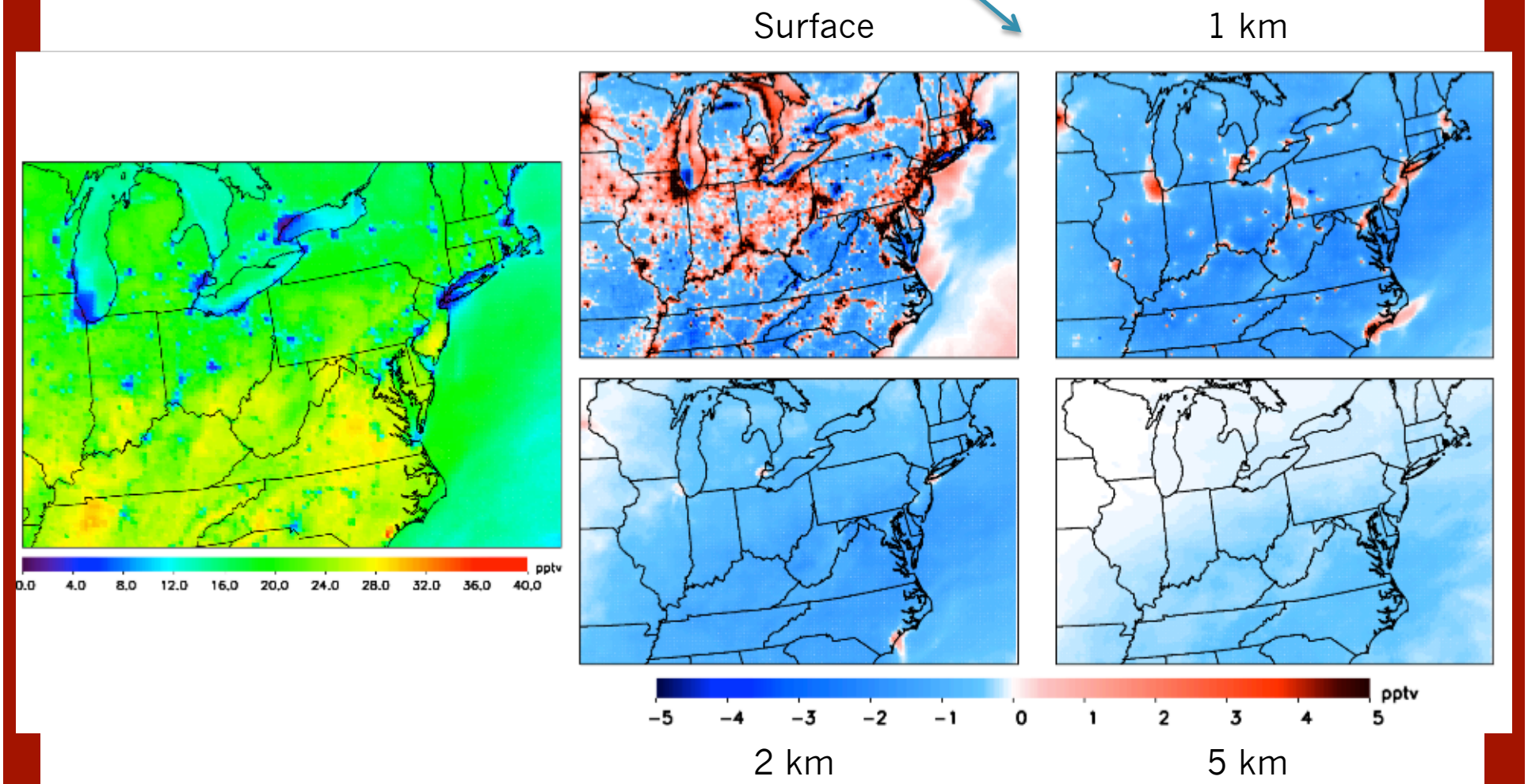
HO_2 Chemistry in the eastern United States

Mean July 2011 daytime (7 AM – 7 PM EDT) HO_2 concentrations



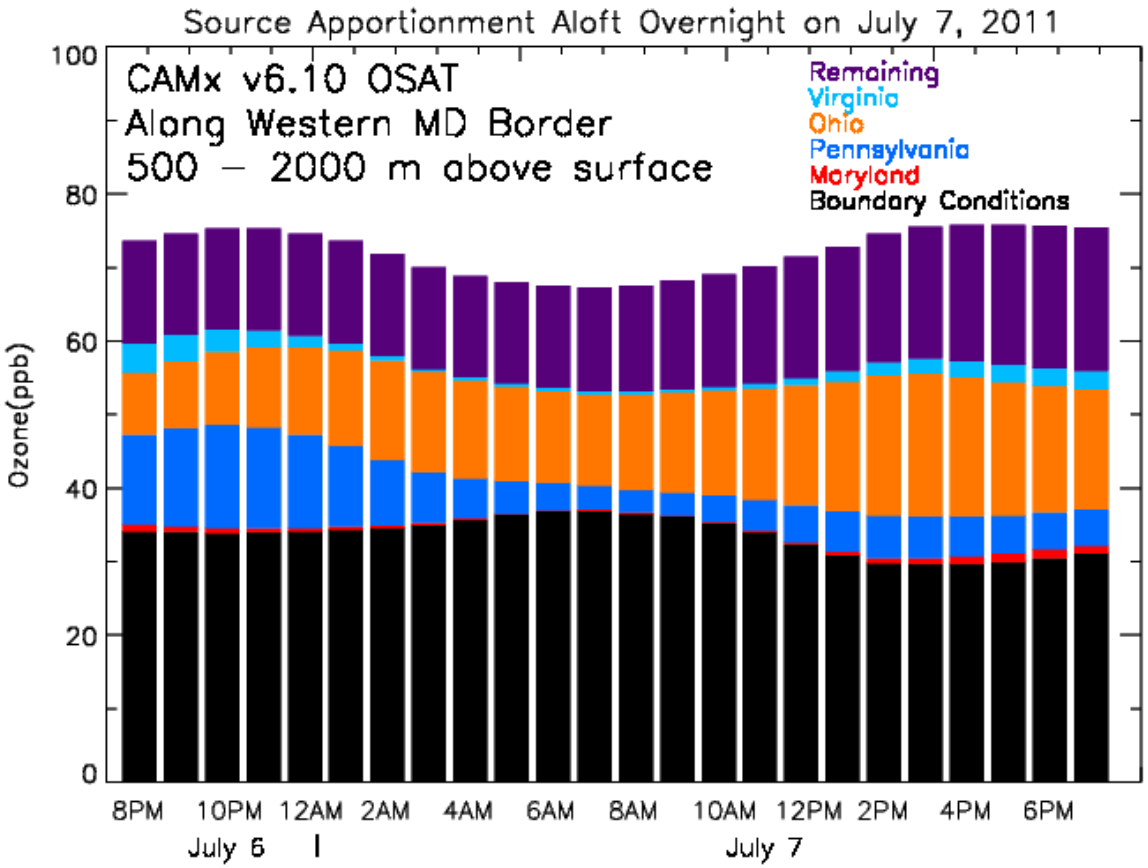
- The $HO_2 + O_3$ reaction can be an important sink of O_x (O_3+NO_2+…) when HO_2 >15 pptv.

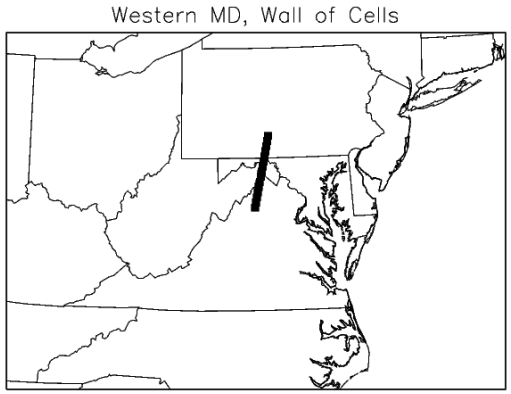
Change in daytime HO_2 concentrations between July 2002 and 2018



- Daytime HO_2 concentrations are decreasing in most areas.
- This is increasing the lifetime of ozone when reaction with HO_2 is important.
- Ozone lifetime with respect to reaction with HO_2 increases from 9.0 to 9.5 days.

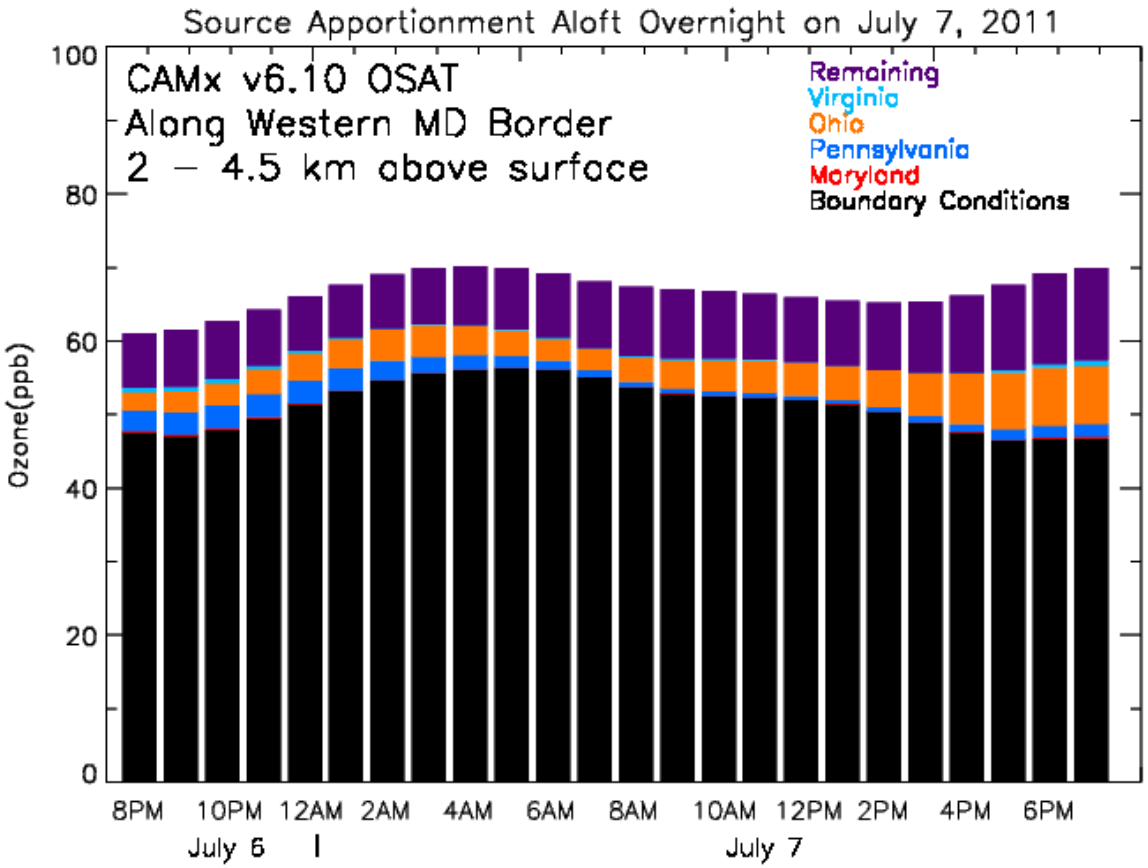
Tagging Ozone Aloft

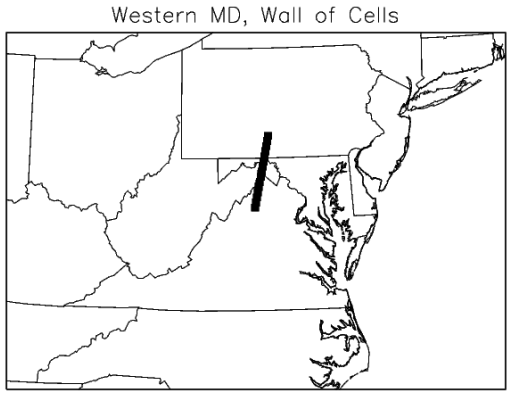




- Between 500 – 2000 m, over 50% of ozone is from the boundary
- Large portion from Ohio

Tagging Ozone Aloft





- Between 2 – 4.5 km above the surface, over 75% of ozone is from the boundary
- Above 4.5 km above the surface (not shown), over 99% of ozone is from the boundary