Scientific Insight from CMAQ modeling for the MDE SIP

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OTC Committee Meeting

“Beta Chemistry”

Problem #1: CMAQ NTR >> observed by NASA DISCOVER-AQ

In standard CMAQ, lifetime of alkyl nitrates (NTR) is ~10 days. Long lifetime means NTR does not contribute to ozone production.

Observations indicate NTR has lifetime of 1 day.

***Solution:* Increase loss of NTR so modeled alkyl nitrates agree with observations taken during the 2011 DISCOVER-AQ campaign.**

***Result:* NTR loss leads to increased NO_x → Ozone increases.**

See Canty et al., Atmos. Chem. Phys. Discuss. 2015

“Beta Chemistry”

Problem #2: Overestimated mobile NO_x Emissions in NEI.

Observed CO/NO_y ratio during the 2011 DISCOVER-AQ is ~1.75 times the NEI. Observed CO in good agreement with NEI → NO_y may be overestimated in NEI.

Solution: **Decrease mobile NO_x emissions by 50%.**

Result: **Lower NO_x concentrations → Ozone decreases. Much better agreement of measured and modeled NO_y.**

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

"Beta Chemistry"

Problem #3: Uncertainties in biogenic emissions modeling

Overall effect on ozone depends on biogenic emissions, especially isoprene.

Solutions: Recent updates to biogenic emissions inventory models MEGAN (v2.04 to v2.10) and BEIS (v3.14 to v3.6*)
**BEIS v3.6 is still under development*

Results:

- **2007 platform: MEGANv2.04 ⟶ MEGANv2.10**
  Overall *decrease* in isoprene → ozone deceases
- **2011 platform: BEISv3.14 ⟶ MEGANv2.10**
  Overall *increase* in isoprene → ozone rises

Modeling Platform and Emissions

- **2011 Modeling Platform**
  - CMAQ v5.0.1 with CB05 and AE5 scheme
  - EPA 2011 meteorology (12 km) in the eastern US

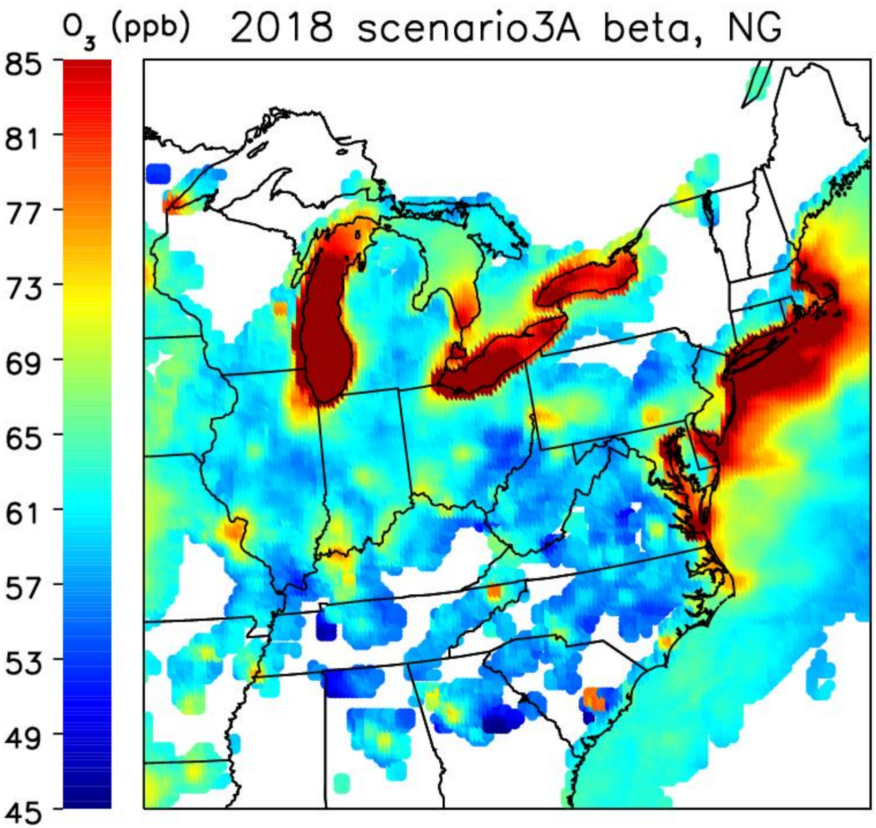
- **2018 Emissions**
  - Optimistic emissions for 2018
  - ICI boiler and EGU NO_x reductions
  - Final Tier 3 mobile reductions

2018 Sensitivity Runs

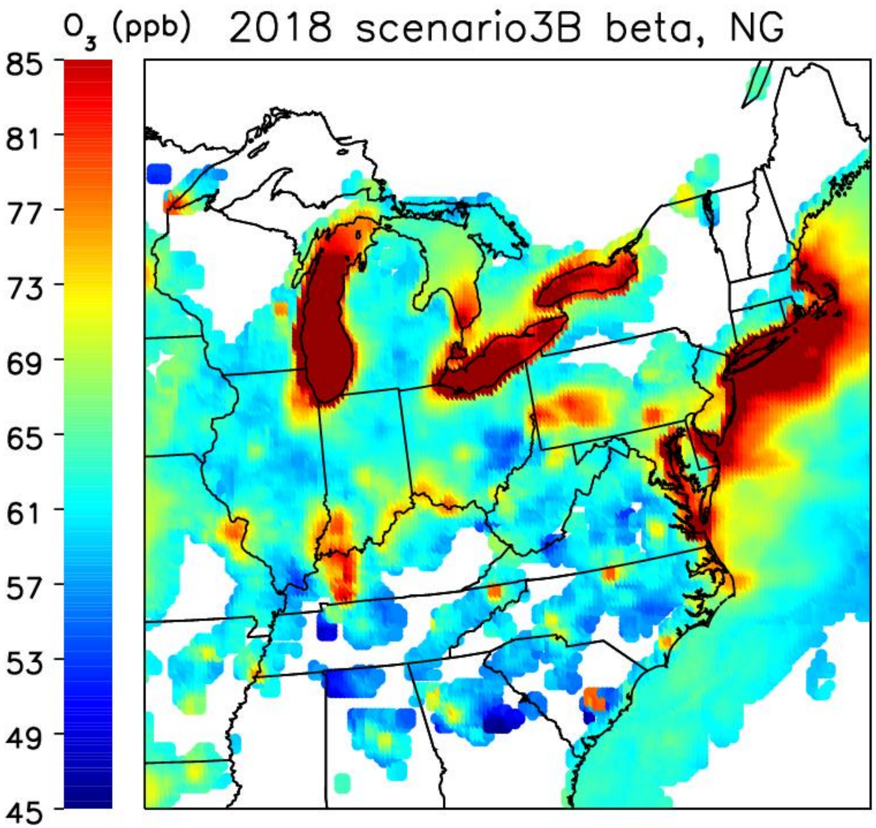
- Adjust power plant (EGU) NO_x
  - IL, IN, KY, MD, MI, NC, OH, PA, TN, VA, WV
- **Scenario 3A → 'best'**
  - Reduce to 2005-2012 best (lowest) CEM observed NO_x rates.
- **Scenario 3B → 'worst'**
  - Increase 3A NO_x to worst (highest) observed NO_x rates
- **Scenario 3C → 'actual'**
  - Increase 3A NO_x to measured 2011 rates.
- **Scenario 3D → 'ideal'**
  - SCRs added to remaining uncontrolled units in neighboring states (VA, IN, KY, OH, MI, NC, OH, VA, WV)
- **Scenario ATT-4 → 'MD extra'**
  - Scenario 3A plus ~50% reduction in MD EGU NO_x

CMAQ Model Beta Scenarios (2011 platform)

"Best Case"- All SCRs Running

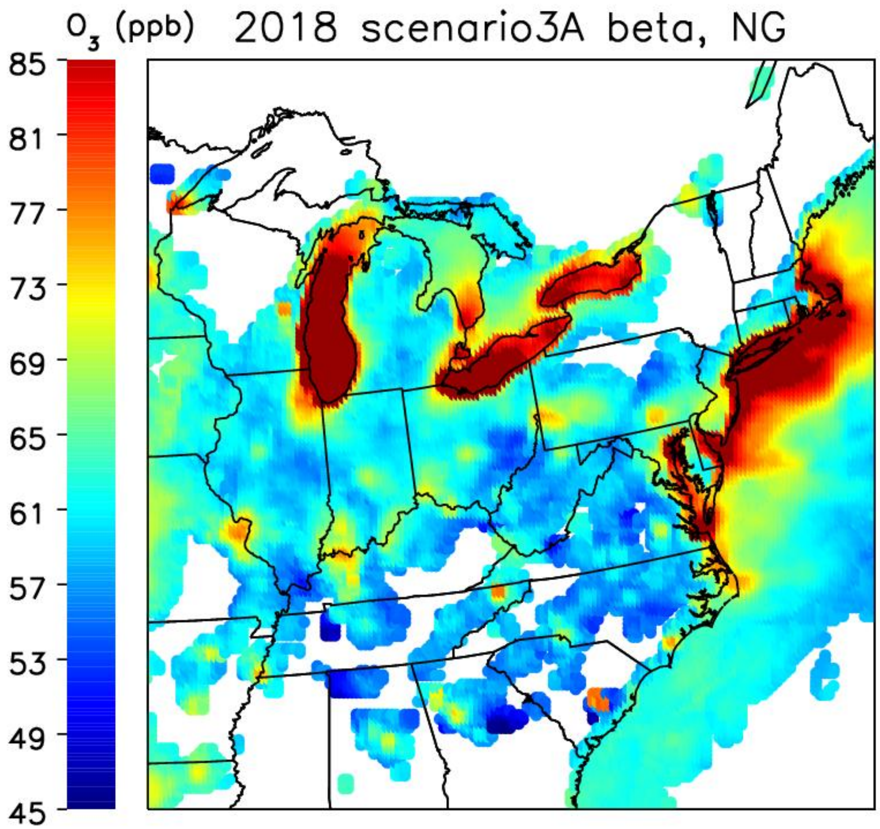


"Worse Case"- No SCRs Running

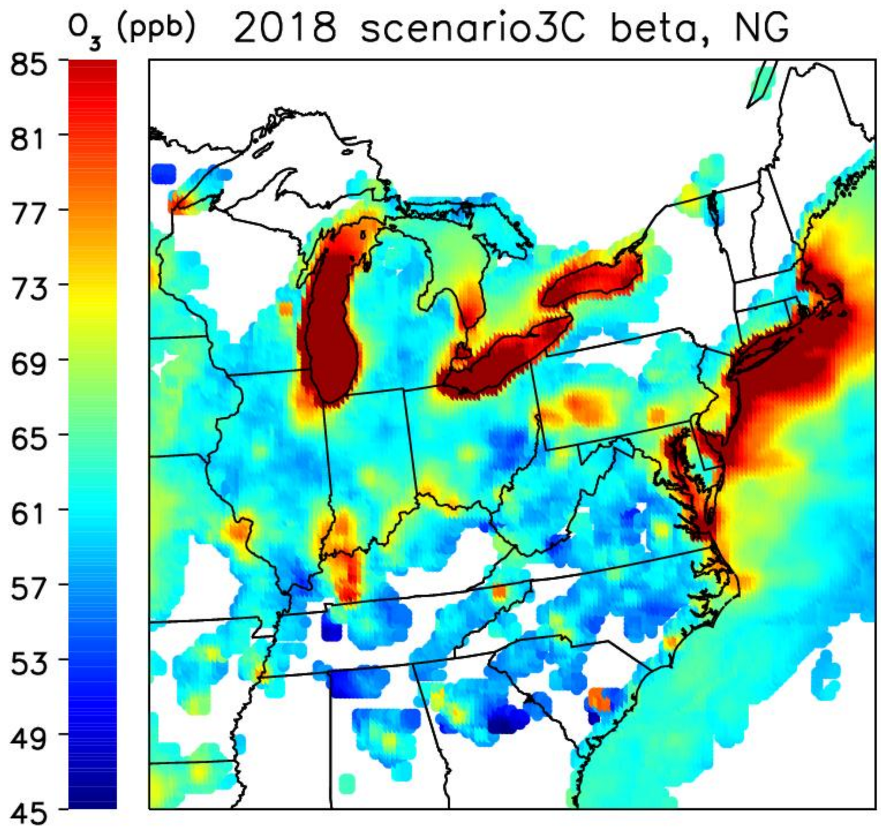


CMAQ Model Beta Scenarios (2011 platform)

“Best Case”- All SCRs Running

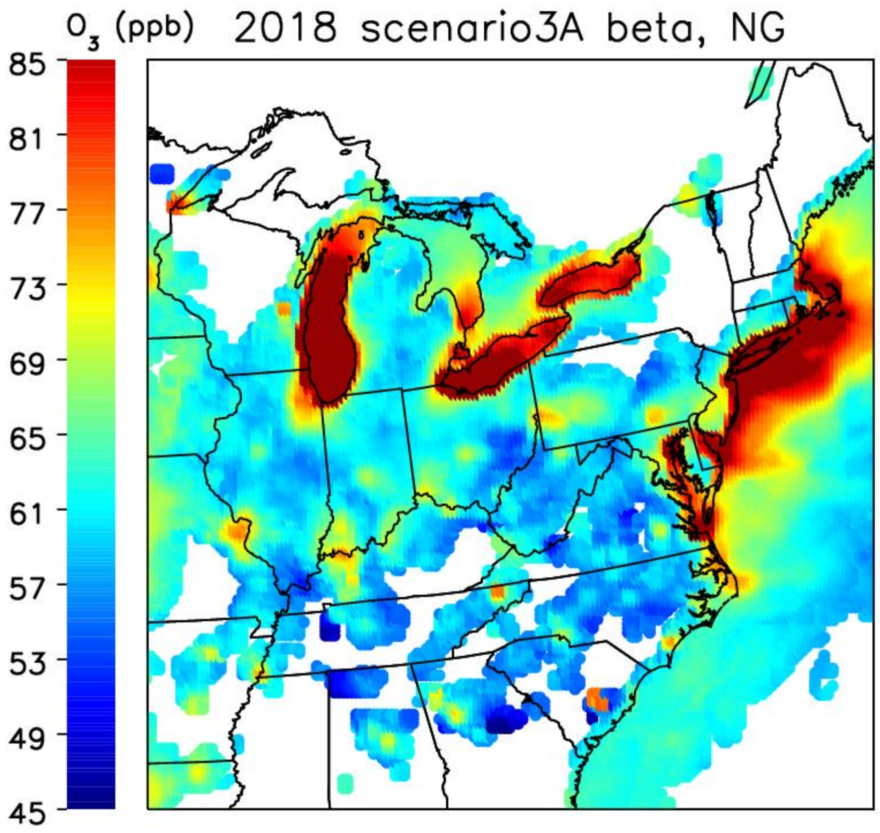


“Real Case”- Some SCRs Running

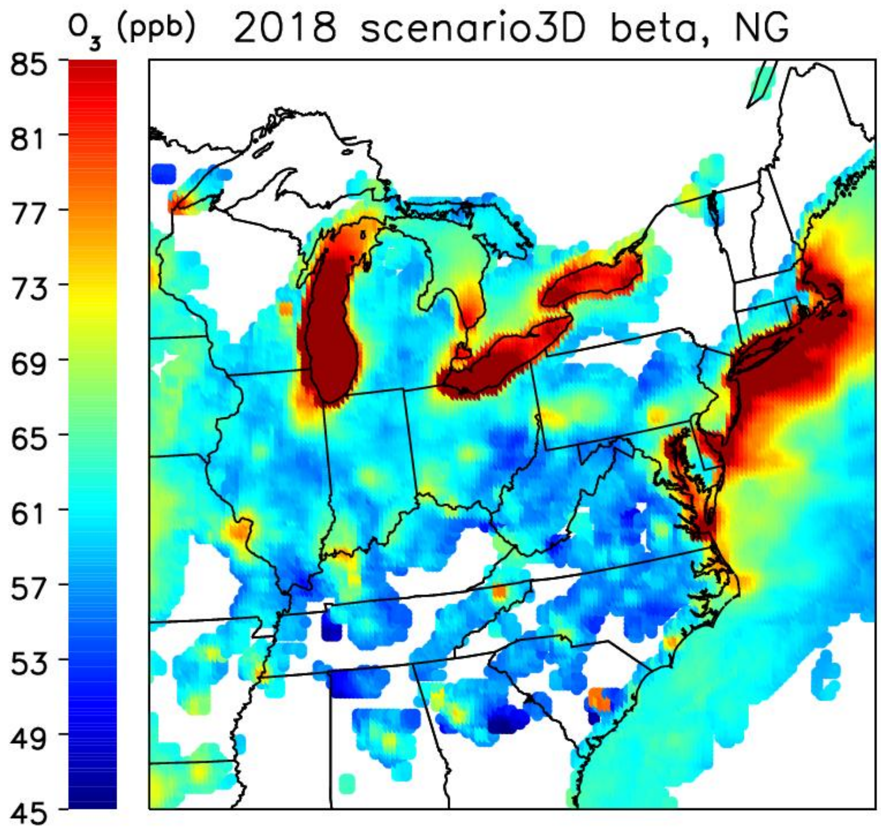


CMAQ Model Beta Scenarios (2011 platform)

"Best Case"- All SCRs Running



"Better Case"- More SCRs Running



All model results for July only (2018): Standard Model

County	Site	DV 2011	DV 2018	3A (ATT-1)	3B	3C	3D	ATT-4
Anne Arundel	Davidsonville	83	68.9	67.9	69.7	69.1	67.6	67.6
Baltimore	Padonia	79	68.2	66.7	69.2	68.4	66.3	66.5
Baltimore	Essex	80.7	69.4	68.3	70.1	69.5	68.0	68.1
Calvert	Calvert	79.7	68.8	67.6	70.4	68.9	67.4	66.4
Carroll	South Carroll	76.3	66.8	65.2	68.7	67.6	64.7	64.8
Cecil	Fair Hill	83	70.0	68.4	71.4	70.4	68.0	68.2
Calvert	S.Maryland	79	66.9	65.7	68.7	67.2	65.4	64.2
Cambridge	Blackwater	75	65.1	64.2	66.0	65.2	63.9	64.0
Frederick	Frederick Airport	76.3	66.9	65.3	68.8	67.7	64.7	64.7
Garrett	Piney Run	72	59.7	58.4	61.5	60.3	55.5	58.4
Harford	Edgewood	90	76.0	74.8	77.0	76.2	74.4	74.5
Harford	Aldino	79.3	66.1	64.8	67.2	66.3	64.5	64.6
Kent	Millington	78.7	65.7	64.3	67.0	66.1	63.9	64.1
Montgomery	Rockville	75.7	64.5	63.6	65.5	64.8	63.2	63.1
PG	HU-Beltsville	79	65.8	64.9	66.7	66.1	64.6	64.5
PG	PG Equest.	82.3	68.6	67.5	69.6	68.8	67.2	67.0
PG	Beltsville	80	66.4	65.4	67.2	66.6	65.1	65.1
Washington	Hagerstown	72.7	63.1	61.8	65.0	64.0	61.0	61.7
Baltimore City	Furley	73.7	63.5	62.5	64.2	63.7	62.3	62.3

All model results for July only (2018): Beta Model

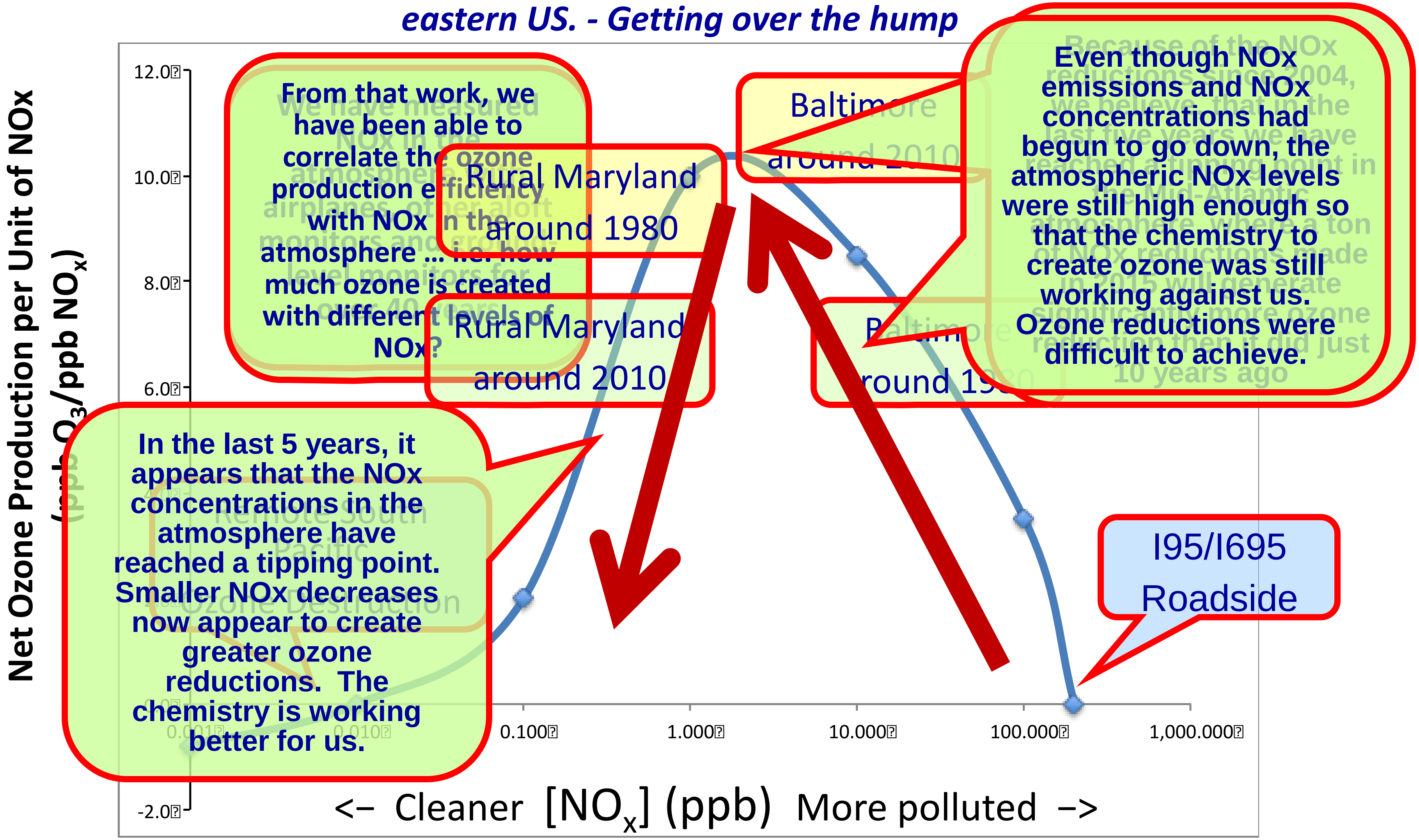
County	Site	DV 2011	DV 2018	3A (ATT-1)	3B	3C	3D	ATT-4
Anne Arundel	Davidsonville	83	70.1	68.9	71.1	70.2	68.6	68.4
Baltimore	Padonia	79	69.4	67.7	70.6	69.7	67.4	67.4
Baltimore	Essex	80.7	68.8	67.4	69.6	68.9	67.1	67.2
Calvert	Calvert	79.7	70.7	69.0	72.5	70.8	68.8	67.6
Carroll	South Carroll	76.3	68.0	65.9	70.4	69.0	65.2	65.4
Cecil	Fair Hill	83	70.0	67.9	72.0	70.7	67.4	67.7
Calvert	S.Maryland	79	67.6	66.2	70.1	67.8	66.0	63.6
Cambridge	Blackwater	75	66.8	65.9	67.6	66.9	65.6	65.7
Frederick	Frederick Airport	76.3	67.9	65.9	70.2	68.8	65.2	65.2
Garrett	Piney Run	72	59.7	58.1	61.7	60.5	54.8	58.1
Harford	Edgewood	90	76.4	74.6	77.6	76.6	74.2	74.3
Harford	Aldino	79.3	66.5	64.7	68.0	66.8	64.3	64.4
Kent	Millington	78.7	66.2	64.4	68.0	66.8	63.9	64.1
Montgomery	Rockville	75.7	64.0	63.1	65.1	64.4	62.7	62.5
PG	HU-Beltsville	79	66.1	65.2	67.1	66.3	64.9	64.8
PG	PG Equest.	82.3	68.8	67.6	69.9	69.0	67.3	67.0
PG	Beltsville	80	67.5	65.8	68.4	67.5	65.6	65.5
Washington	Hagerstown	72.7	64.2	62.4	66.8	65.6	61.4	62.3
Baltimore City	Furley	73.7	62.9	61.6	63.7	63.1	61.4	61.5

Modeling Preliminary EPA Problem Areas

County, State	AQS #	Design Value 2011	DV 2018	DV S3A	DV S3B	DV S3C	DV S3D	DV ATT4
Attainment Problems - 2018								
Harford, MD	240251001	90.0	76.3	74.6	77.6	76.6	74.2	74.3
Fairfield, CT	090013007	84.3	73.0	72.5	73.3	73.1	72.4	72.5
Fairfield, CT	090019003	83.7	75.6	75.2	75.9	75.7	75.2	75.2
Suffolk, NY	361030002	83.3	73.6	73.1	73.8	73.6	73.1	73.1
Maintenance Problems - 2018								
Fairfield, CT	090010017	80.3	72.3	72.0	72.5	72.4	71.9	71.9
New Haven, CT	090099002	85.7	74.8	74.5	75.0	74.8	74.4	74.4
Camden, NJ	340071001	82.7	72.4	71.1	73.5	72.9	70.9	71.1
Gloucester, NJ	340150002	84.3	73.8	72.3	75.3	74.4	72.0	72.1
Richmond, NY	360850067	81.3	73.7	72.9	74.1	73.7	72.8	72.9
Philadelphia, PA	421010024	83.3	72.3	70.7	73.7	72.8	70.3	70.6

Have We Reached a Tipping Point with NO_x?

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



Conclusion

- ‘Beta chemistry’ can improve CMAQ simulations of ozone precursors, and predict slightly higher ozone.
  - More difficult to achieve attainment with expected mobile source emissions reductions.
  - Bigger improvements from power plant emissions.

- Ozone production efficiency: Having reached the tipping point, emissions controls in the future should lead to greater improvements of ozone per ton of NO_x.

Extra Slides

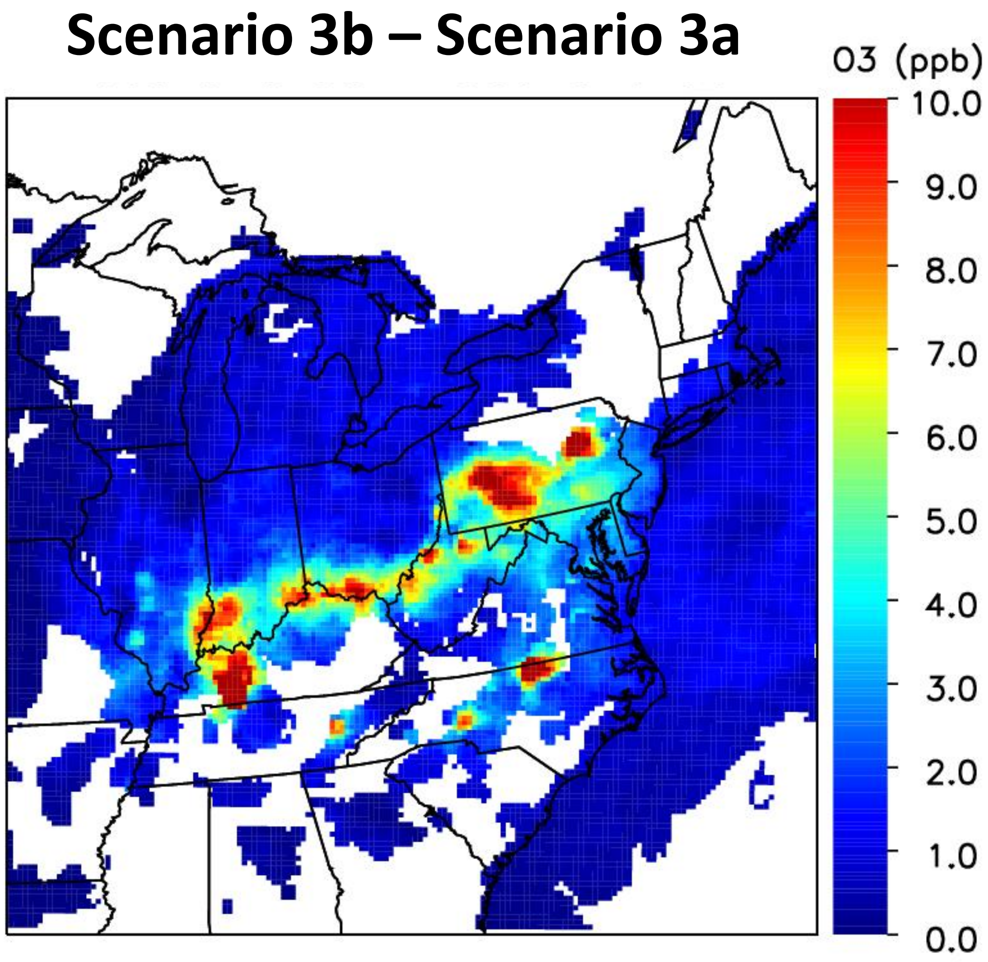
New DV Guidance

- Find maximum baseline O_3 of 3x3 grid for each cell.

- Max. O_3 for future case at same point as baseline case

- Calculate mean for 10 highest days above 75 ppb
 (5 day, 60ppb min)

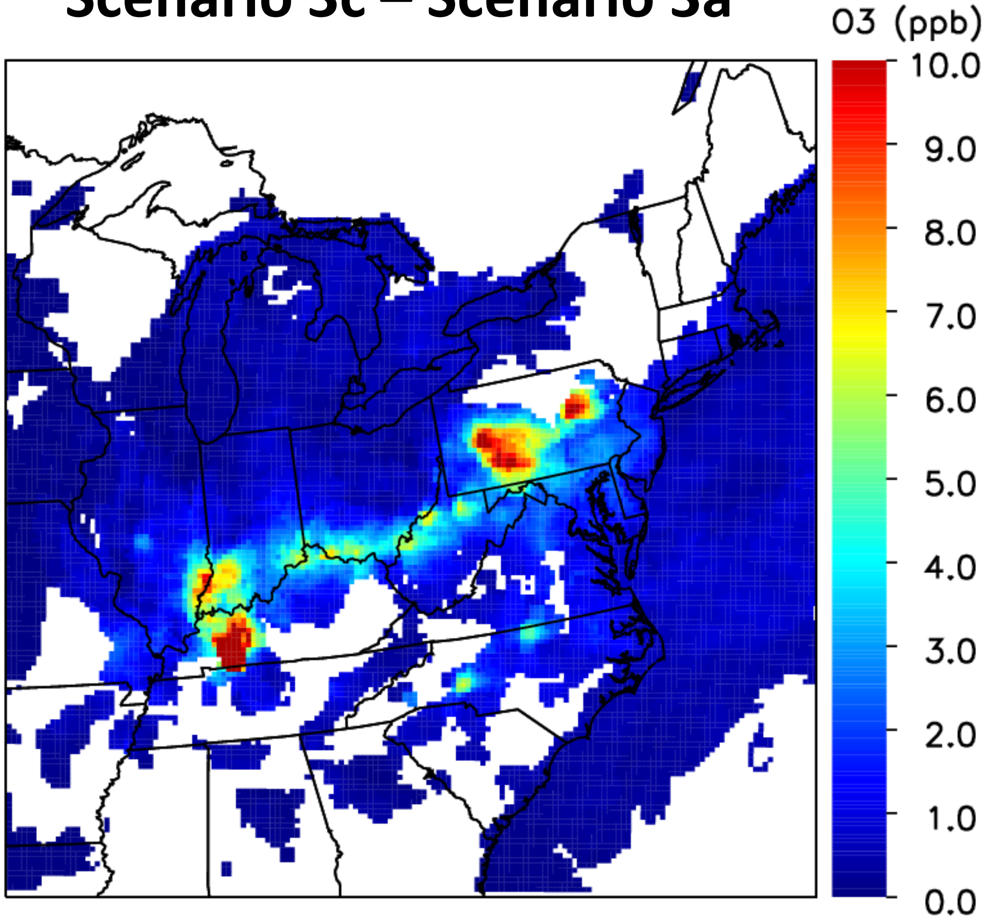
CMAQ Model Beta Scenarios (2011 platform)



3a: best case
3b: worst case

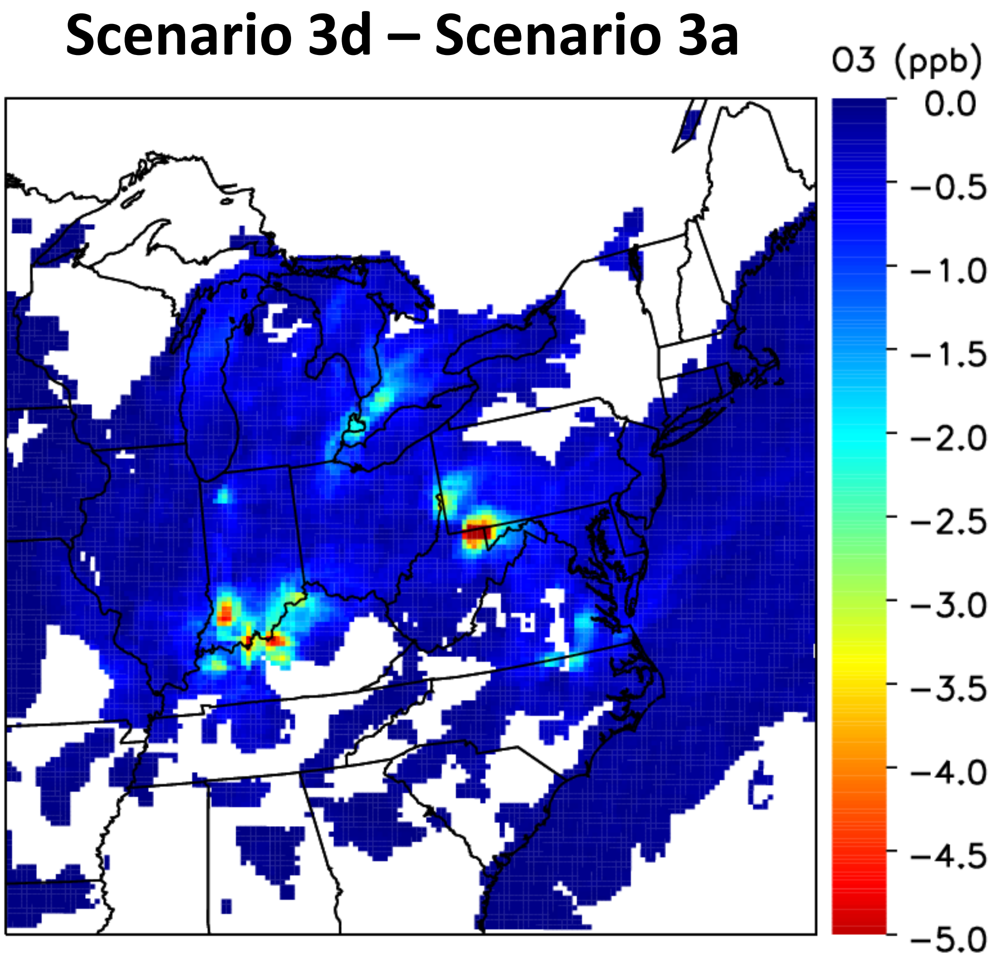
CMAQ Model Beta Scenarios (2011)

Scenario 3c – Scenario 3a



3a: best case
3c: actual case

CMAQ Model Beta Scenarios (2011)



3a: best case
3d: ideal case

The color bar is different!

Notes

On Ozone Production Efficiency Diagram

1. This shows net ozone production per unit NOx.
2. It peaks somewhere around 1 ppb NOx; ozone is still made faster at higher NOx concentrations, but the rate of increase tails off.
3. Boxes fly in to show where urban Baltimore was in the ~1980 and in 2010. Ozone improved between 1980 and 2010, but slowly because as NOx concentrations fell the efficiency increased. We moved left but also up.
4. Now the city is getting over the hump and rural areas (next two fly ins) are definitely in the range where small improvements in NOx emissions can mean big improvements in O3.
5. The other side of that coin is any backsliding will bring big problems.
6. The last fly-ins are to show that under extremely high concentrations ozone is all tied up as NO2 – but the NO2 is toxic. At the other extreme, natural processes destroy ozone but American cities will probably never be as clean as tropical islands.