Dynamic evaluation of the CMAQv5.0 modeling system: Assessing the model's ability to simulate ozone changes due to NO_x emission reductions

Kristen M. Foley
USEPA

International Technical Meeting on
Air Pollution Modeling and its Application
August 29th 2013

Acknowledgements

- EPA: Christian Hogrefe, George Pouliot, Shawn Roselle, Norm Possiel, Heather Simon, Brian Timin, Jim Godowitch, Rob Gilliam, Wyat Appel, Rob Pinder, Sharon Philips, Kirk Baker, Alexis Zubrow, Alison Eyth, Barron Henderson (now at Univ. of FL), Farhan Akhtar (now at US State Dept.)

- CSC: Lucille Bender, Ryan Cleary, Allan Beidler,

Dynamic Evaluation of Air Quality Models

- **Motivation:** Air quality models are used to determine the impact of different emission reductions strategies on ambient concentration levels.

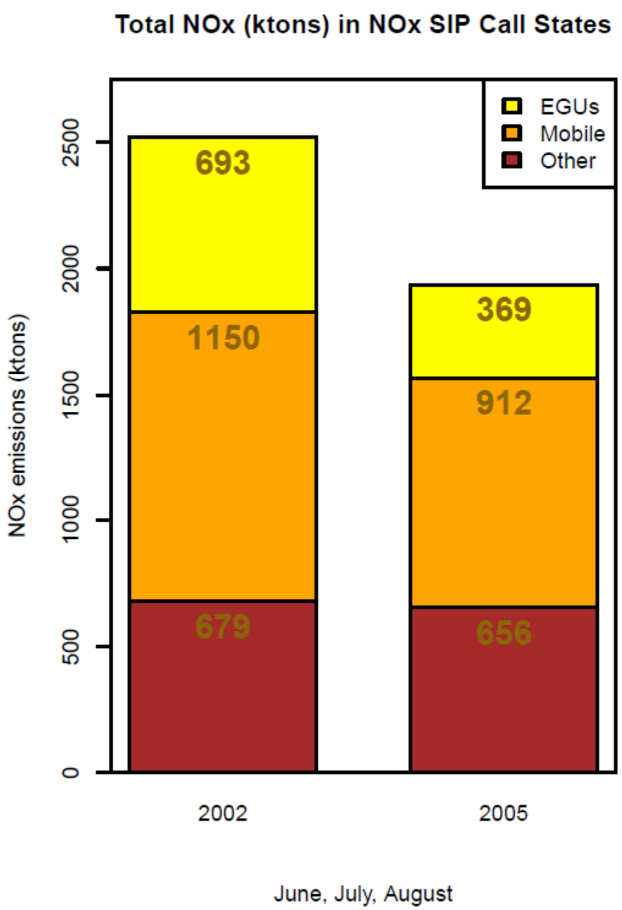
- **Dynamic Evaluation:** Evaluating the model's ability to predict changes in air quality given changes in emissions (or meteorology).

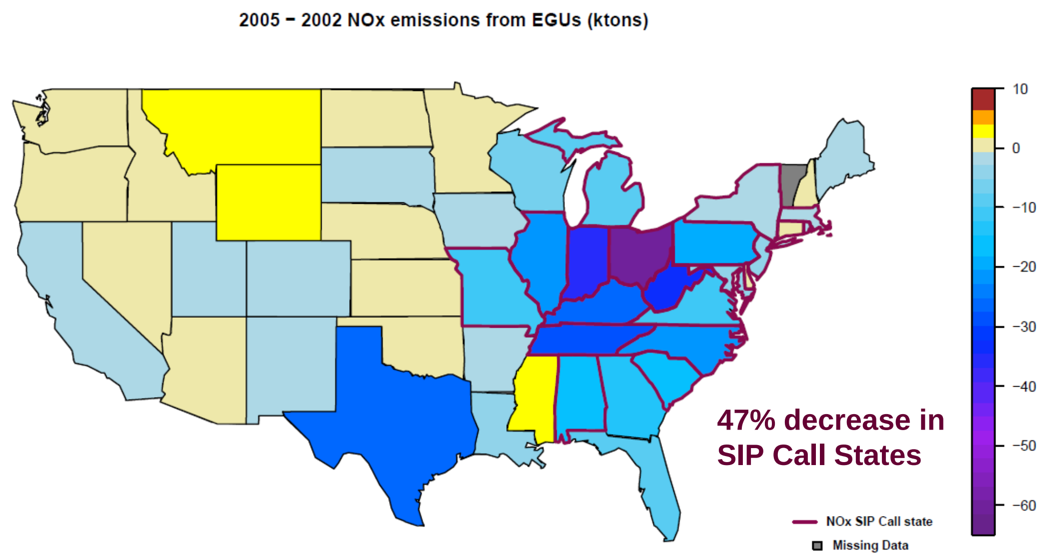
- Dynamic evaluation is only possible if a retrospective case ("natural experiment") exists where:
  1. substantial emission reductions have resulted in discernible changes in air quality over time and
  2. the change in emissions can be quantified accurately.

- An additional challenge is that the air quality changes over time are also driven by meteorological variability.

foley.kristen@epa.gov

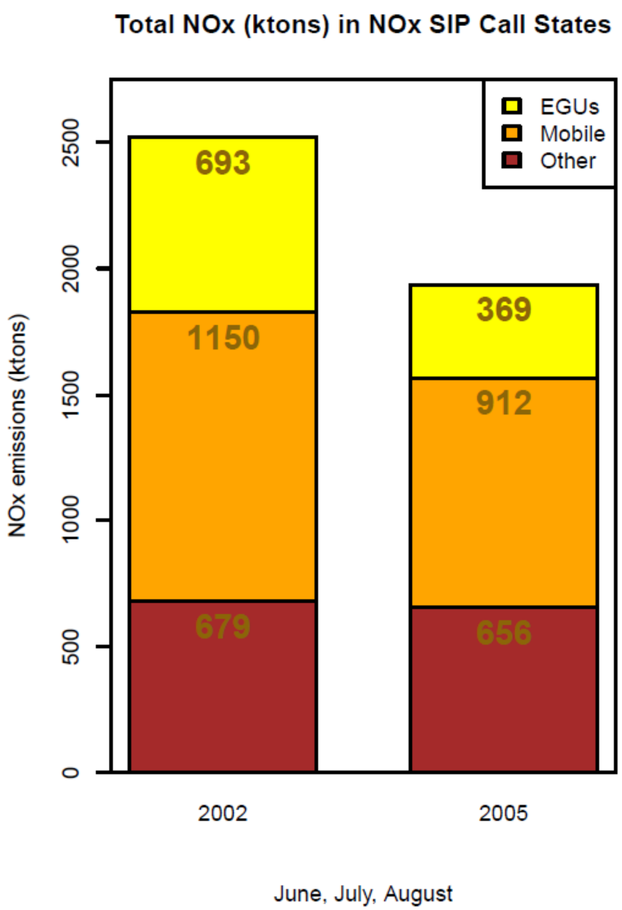
NO_x SIP Call
EPA's Nitrogen Oxides State Implementation Plan



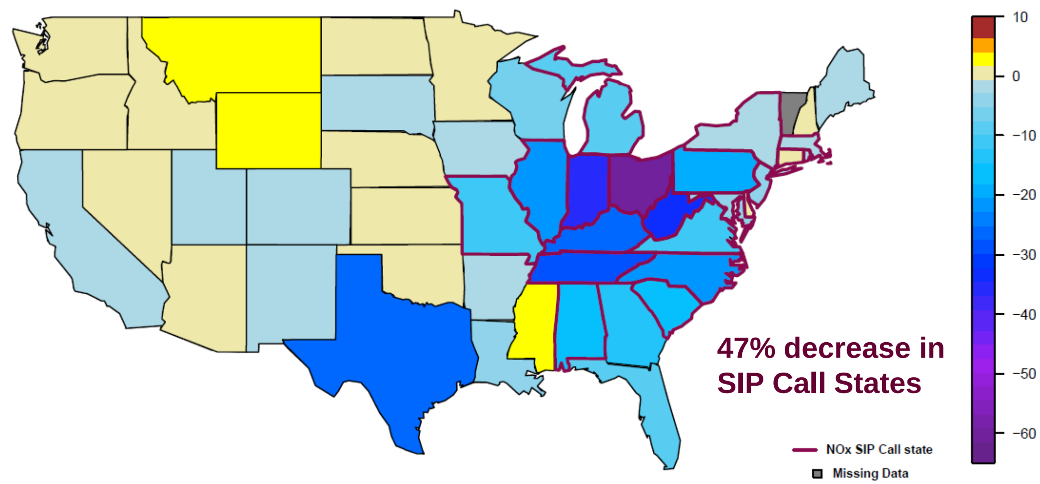


- Reductions were made to EGU emissions in the Eastern US, resulting in 30% reduction in ozone in some parts of the region.
- Continuous emissions monitoring (CEM) data available for major units, allowing for accurate quantification of the emission reduction.

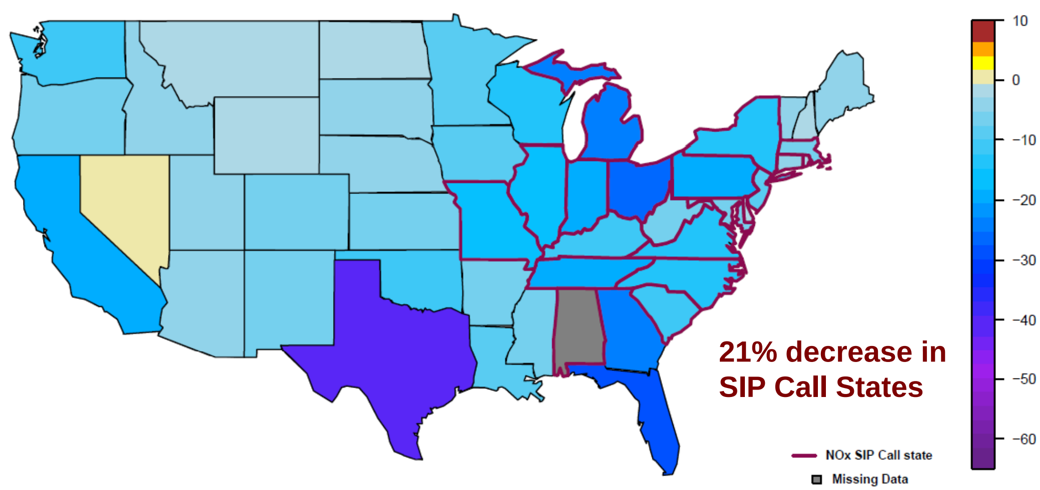
NO_x SIP Call
EPA's Nitrogen Oxides State Implementation Plan



2005 − 2002 NOx emissions from EGUs (ktons)



2005 − 2002 NOx emissions from Mobile sources (ktons)



Recent dynamic evaluation studies

Gilliland et al. (2008) – Evaluation of CMAQv4.6 for 2002, 2005

"The evaluation results presented in this study suggest that the air quality model predictions underestimate the O_3 reductions observed after the NO_x SIP Call was implemented."

Godowitch et al. (2011) – Evaluation of CMAQv4.7 for 2002-2006

Underestimation of decrease in weekday morning NO_x levels and max 8hr average ozone levels in urban areas may be due to underestimation of trends in non-mobile surface NO_x emissions.

Napelenok et al. (2011), Zhou et al. (2013), Kang et al. (2013)
DDM and brute-force sensitivity analyses for CMAQv4.7 for 2002 and 2005/2006

Modeled ozone response can be improved by adjusting ground-level NO_x emissions inputs, but adjusted ozone predictions still under-estimate observed reductions.

foley.kristen@epa.gov

Dynamic Evaluation of CMAQ Version 5

- **Model description:**
  - CMAQ: CMAQv5.0.1 with updated bidirectional NH_3 exchange code (bidi1.3) and inline photolysis, 35 layers with 20m first layer, CONUS 12km US1 domain.
  - Meteorology: WRFv3.3, MCIPv4.0
  - Emissions: SMOKEv3.1, MOVESv2010b for 2002 and 2005,
    Inline NO produced from lightning using year specific data from NLDN,
    BELD3 land use for gridded fractional crop distributions,
    BEISv3.1.4 for inline biogenics,
    NLCD 2001, 50 category land use data,
    Fertilizer emissions from EPIC simulation with latest EPA updates using 2002 fertilizer sales.
  - Boundary conditions: 2005 monthly median values from GEOS-Chem v9-01-02 simulation using v8-02-01 chemistry, GEOS-5 meteorology, and ICOADS shipping emissions.

- **Two kinds of simulations:**
  - **Evaluation runs** allow for operational and dynamic evaluation of June-August 2002 and 2005 predictions compared to observations.
  - **"Cross" simulations** allow for isolation of the impact on the ozone predictions from (a) changes in emissions only or (b) changes in meteorology only.

foley.kristen@epa.gov

Updates from v4.6 to v5.0.1 related to dynamic evaluation of ozone

Meteorology

- Change from MM5 to WRF meteorology. ↑ O_3 in the southeast
- Updated data assimilation in WRF improves O_3 transport in the north east. ↓ O_3

Emissions

- New mobile emissions model MOVES incorporates latest emissions data and increases NO_x emissions (esp. light and heavy-duty trucks) by 30%. ↑ O_3 ↓ O_3 in urban areas
- New modeled NO_x source aloft: NO produced from lightning. ↑ O_3

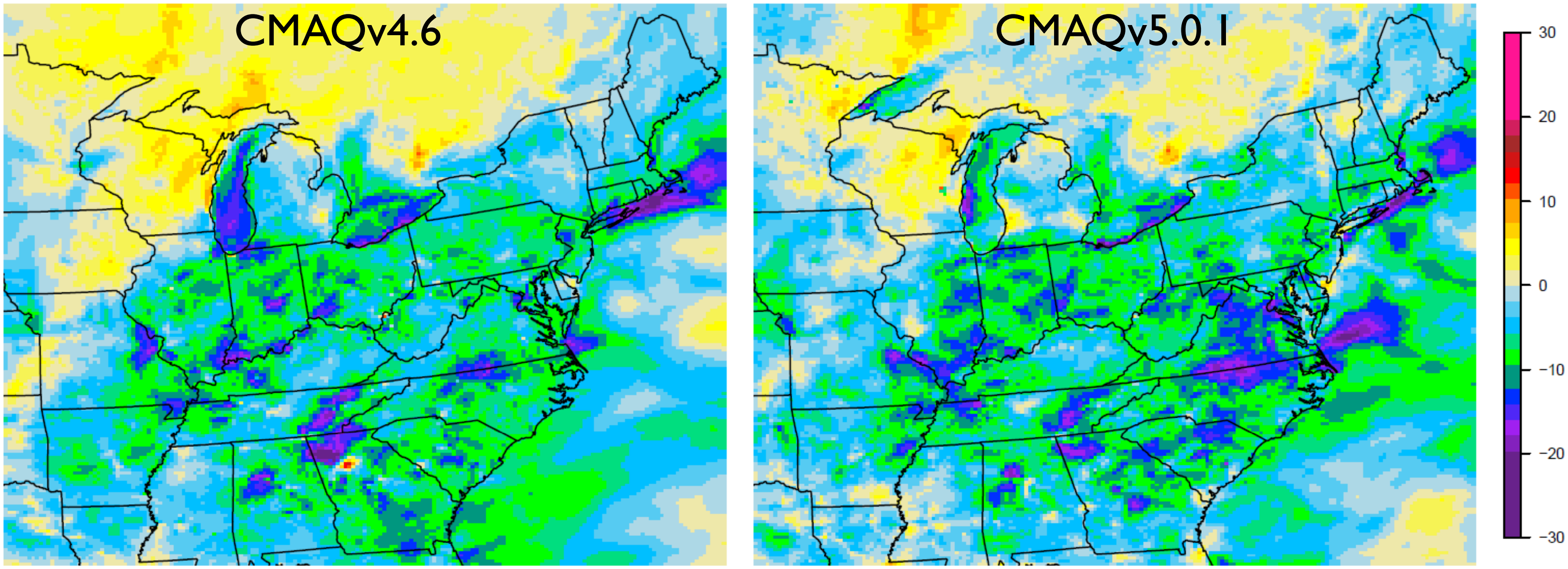
CMAQ

- Updates to CMAQ photolysis algorithm incorporate effects of aerosol loading on photolysis rates. ↓ O_3 in urban areas
- 35 vertical layers with a 20m first layer (compared to 14 vertical layers). ↓ O_3
- More realistic boundary conditions from a global model (GEOS-Chem) compared to fixed profiles. ↑ O_3

→ Ozone increases an average of ≈ 2ppb (4%) from v4.6 to v5 in both 2002 and 2005.

foley.kristen@epa.gov

2005 - 2002 Change in high summertime ozone (ppb)

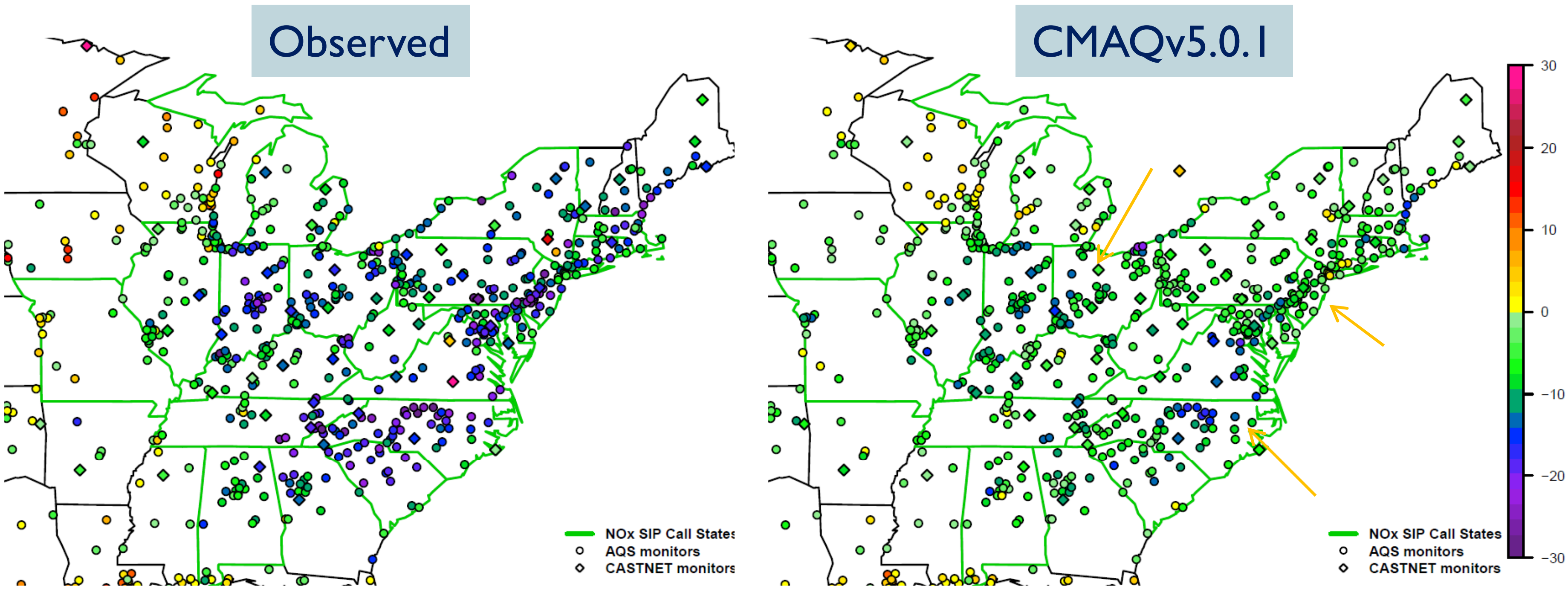


The model metric used for attainment demonstrations is based on an average of "high" summertime max 8-hr average ozone days (MDA8 O_3).

Here we focus on the **average of the top 10 summer MDA8 O_3** values.

foley.kristen@epa.gov

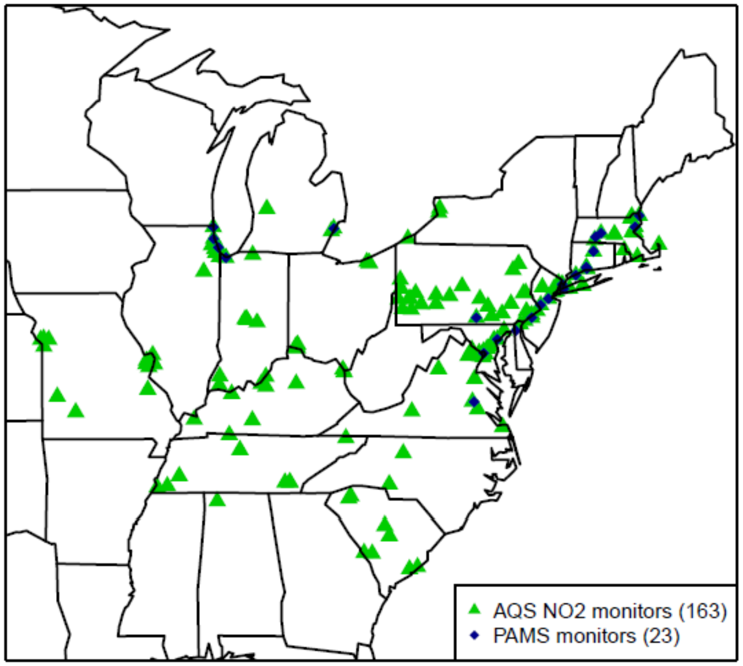
2005 - 2002 Change in high summertime ozone (ppb)

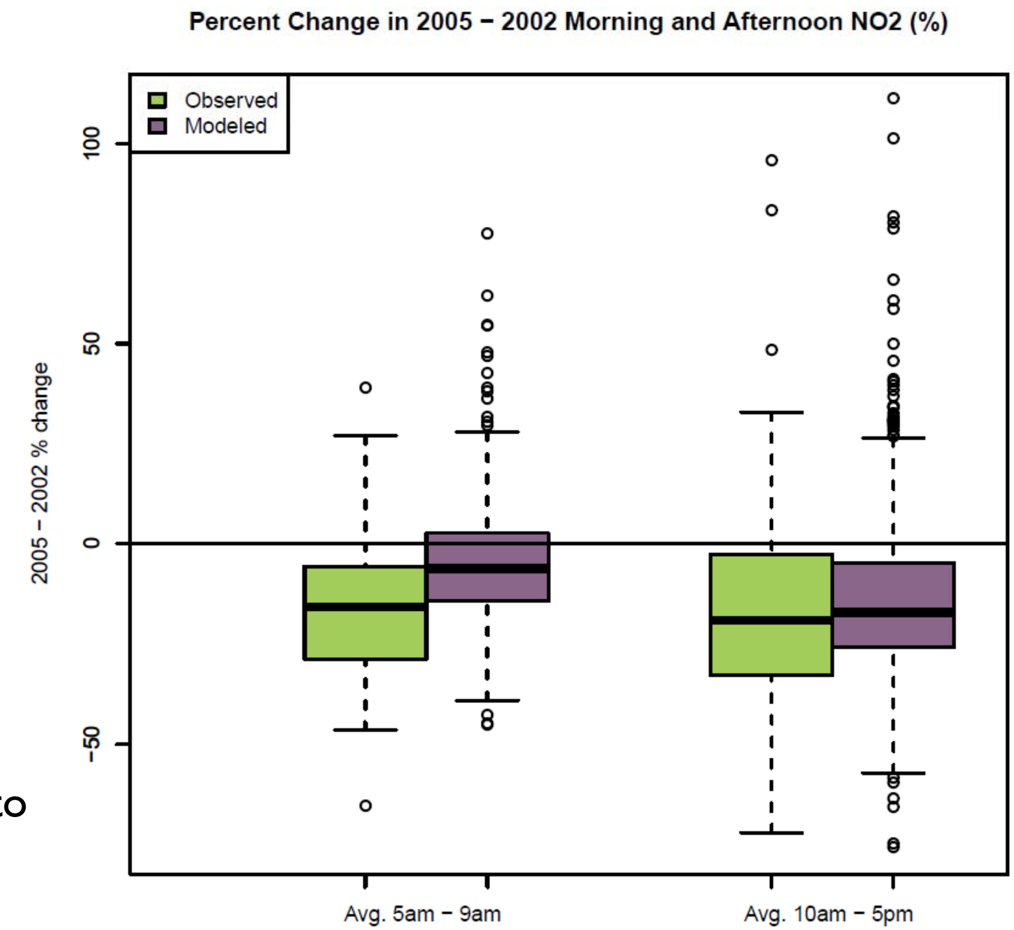


- Model predicts large decreases in NC and VA, but not large enough.
- Model misses region of 15-25ppb decrease along east coast and Ohio River Valley.

foley.kristen@epa.gov

The usual suspects….
Percent change in 2005 – 2002 weekday NO_2





- Morning NO_x concentrations have been shown to be strongly related to ground level NO_x emissions levels.
- Decrease in NO_2 mixing ratios is underestimated in early morning hours.

foley.kristen@epa.gov

Creation of "Cross" Simulations

	2002 Emissions 2002 Meteorology	2005 Emissions 2005 Meteorology
2002 Emissions 2005 Meteorology	*Meteorology change*	*Emissions change*
2005 Emissions 2002 Meteorology	*Emissions change*	*Meteorology change*

"Cross" simulations allow for isolation of the impact on the ozone predictions from (a) changes in emissions only or (b) changes in meteorology only.

foley.kristen@epa.gov

Creation of "Cross" Simulations

- The processing of emissions from EGUs **with available monitoring (CEM) data** in both 2002 and 2005 is based on **unit specific adjustments** of the emissions to account for the impact of different meteorological influences in a different year.

- **Mobile emissions** are based on MOVES simulations using the designated emissions year and meteorology year (e.g. 2002 emissions with 2005 meteorology).

- Emissions from small EGUs without CEM data use the ***emissions year*** for the annual to month factors and meteorology for the month to day factors.

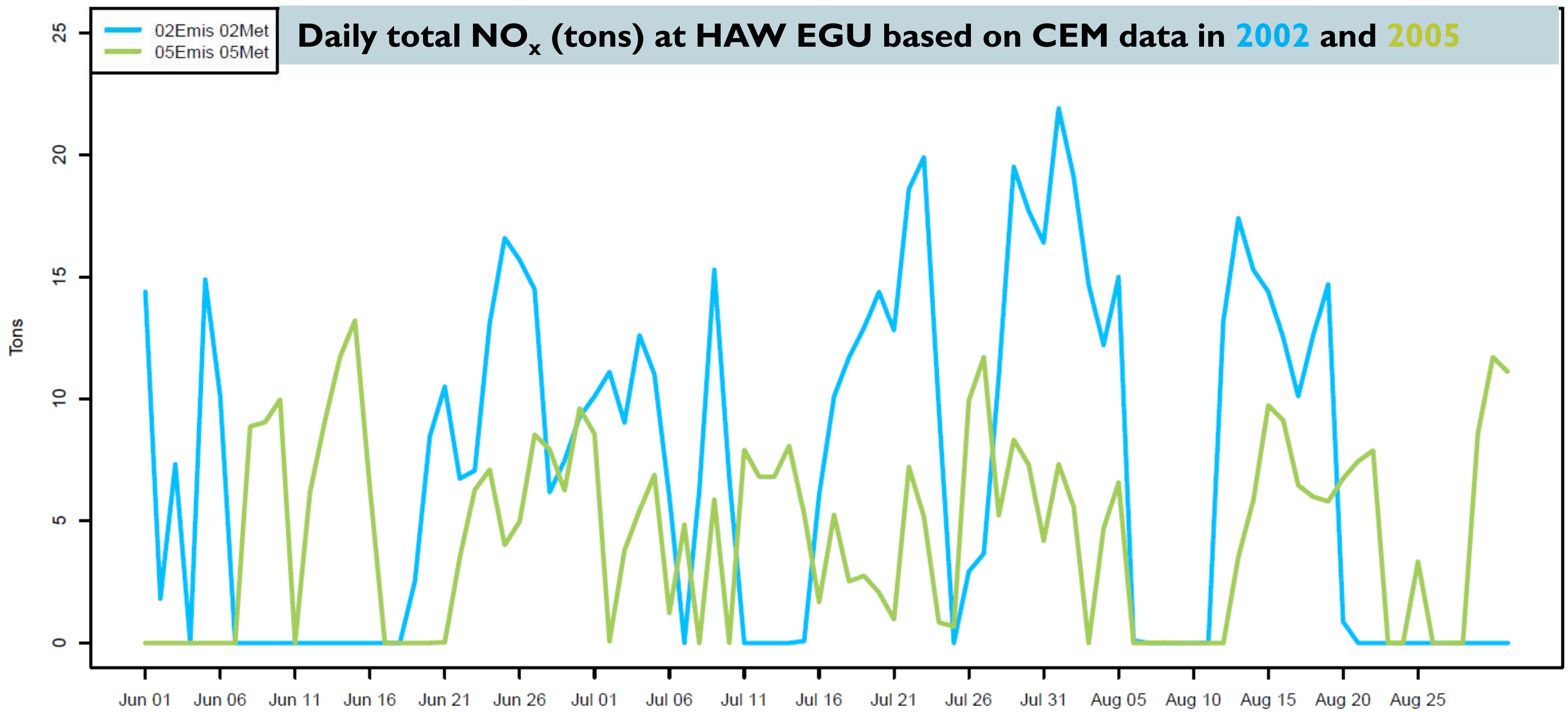
- Emissions from nonroad (e.g. construction), industrial point and large marine sectors are based on the ***emissions year*** but shifted to match the day-of-the week of the meteorology year.

- Emissions from fertilizer application, biogenic sources, NO_x from lightning, fires and dust are tied to the ***meteorological year***.

- All other sectors have the ***same inventory for all scenarios*** except modified for day-of-the-week of the meteorology year.

foley.kristen@epa.gov

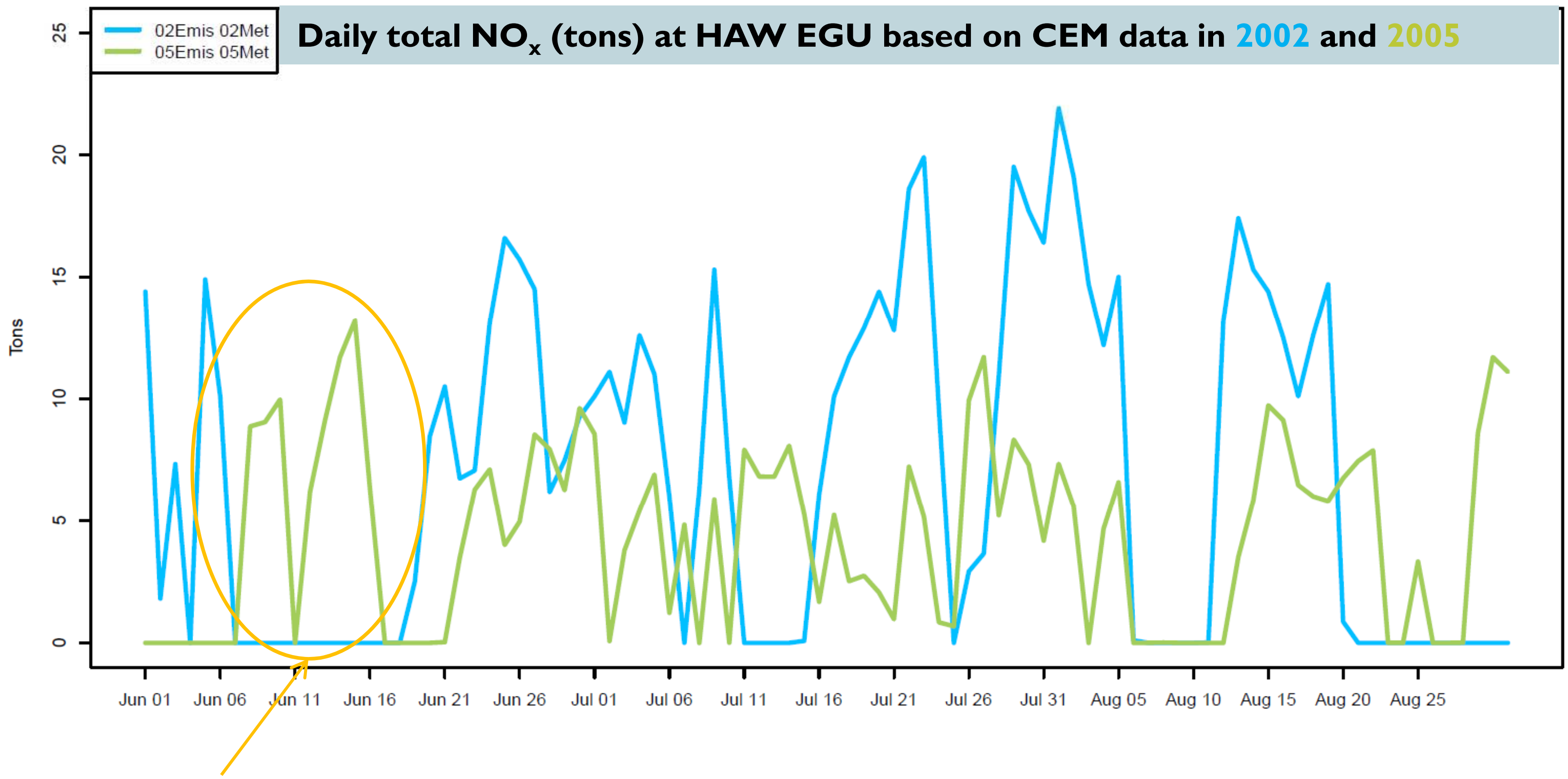
Creation of "Cross" Simulations



- Summertime 2005 NO_x emissions are generally lower than 2002 emissions but the temporal fluctuations are different due to differences in electricity demand which is heavily influenced by year-specific meteorology.

foley.kristen@epa.gov

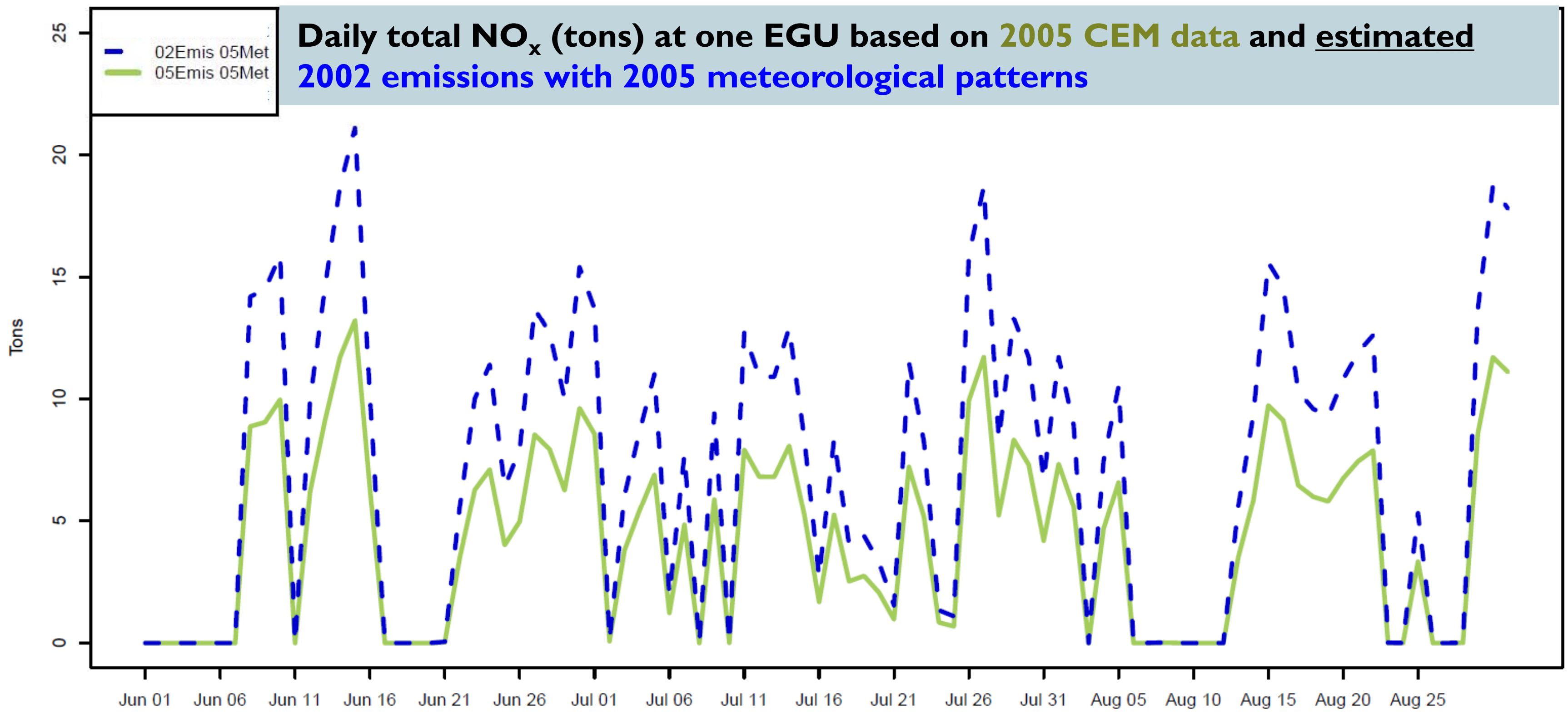
Creation of "Cross" Simulations



- We do not want to simply use the 2002 CEM data with 2005 meteorology inputs to create a cross simulation.
- Such an approach would apply zero NO_x emissions during these high demand days.

foley.kristen@epa.gov

Creation of "Cross" Simulations

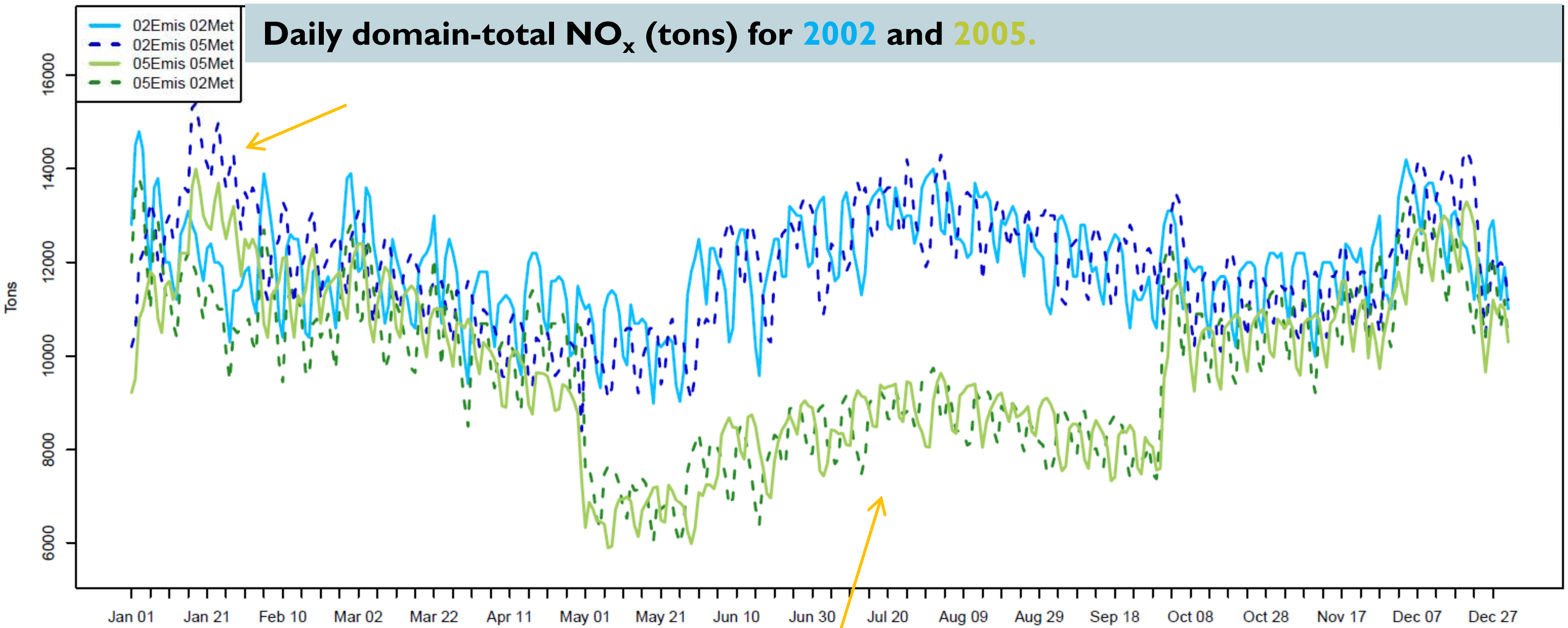


- Instead we scale the hourly 2005 CEM emissions based on the ratio of summer total CEM emissions (S_{Y1}/S_{Y2}) for a particular EGU unit in 2002 versus 2005.

Unit specific calculation: $EMIS_{02e05m} = HRLY\_CEM_{2005} * (S_{2002}/S_{2005})$

foley.kristen@epa.gov

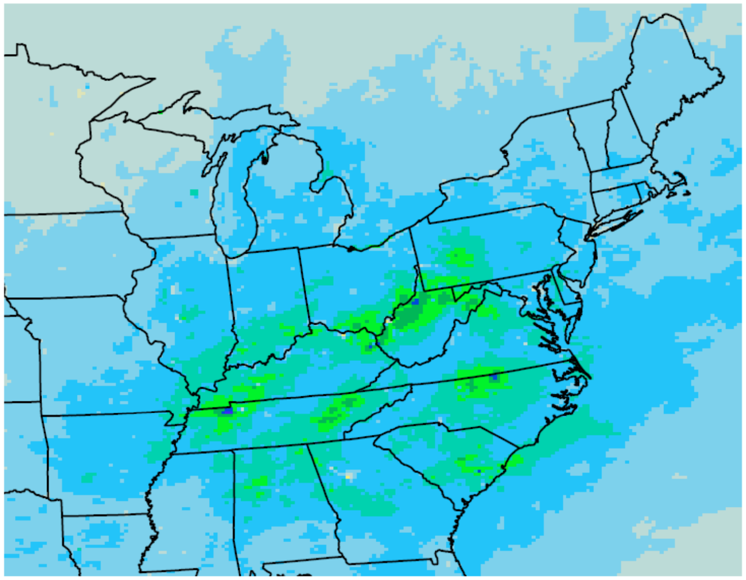
Daily Domain-Total NOx (tons) from CEM Data



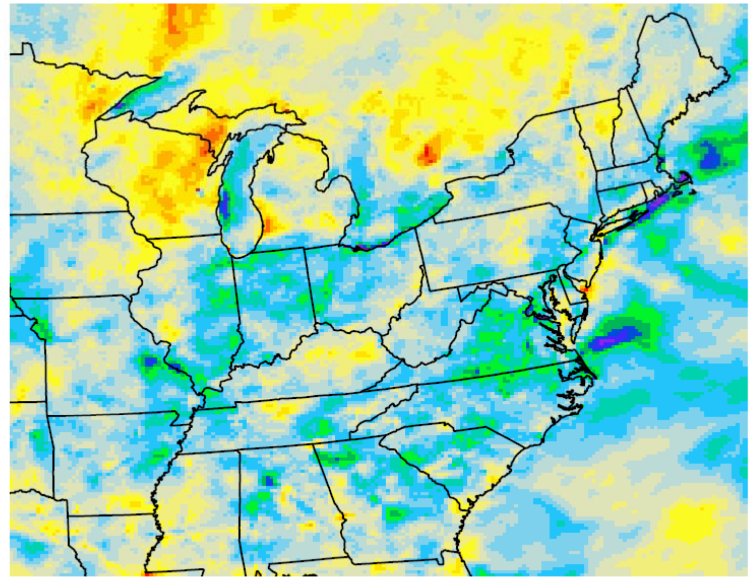
- Summertime change in NO_x emissions from 2002 to 2005 is driven by NOx SIP call emission reductions rather than by changes in meteorology.
- Peak NO_x emissions in January are driven by 2005 meteorology (colder temperatures) rather than by seasonal emission totals.

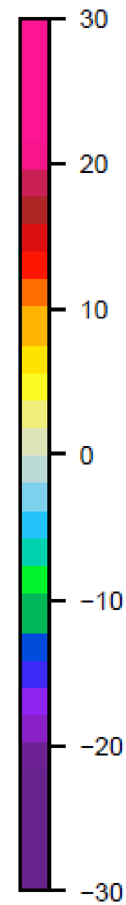
foley.kristen@epa.gov

Change in high ozone due to change in EMISSIONS (with 2002 meteorology)



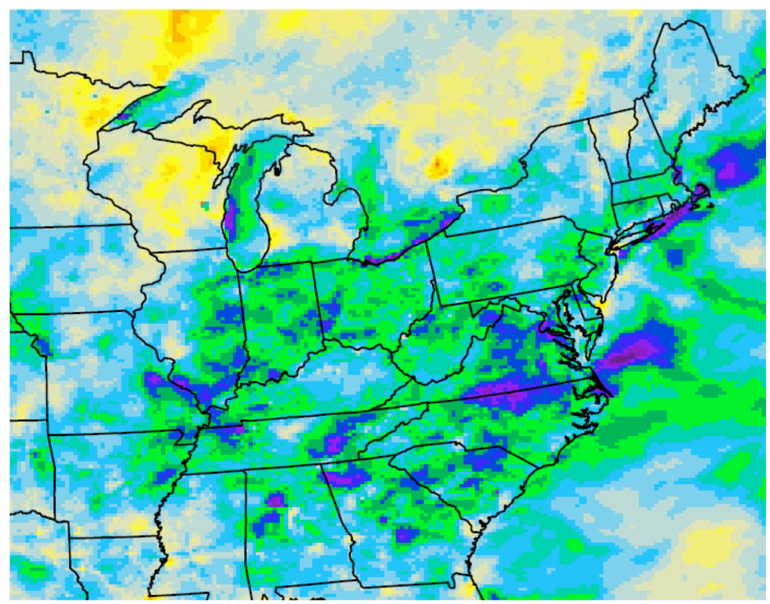
Change in high ozone due to change in METEOROLOGY (with 2002 emissions)





\+

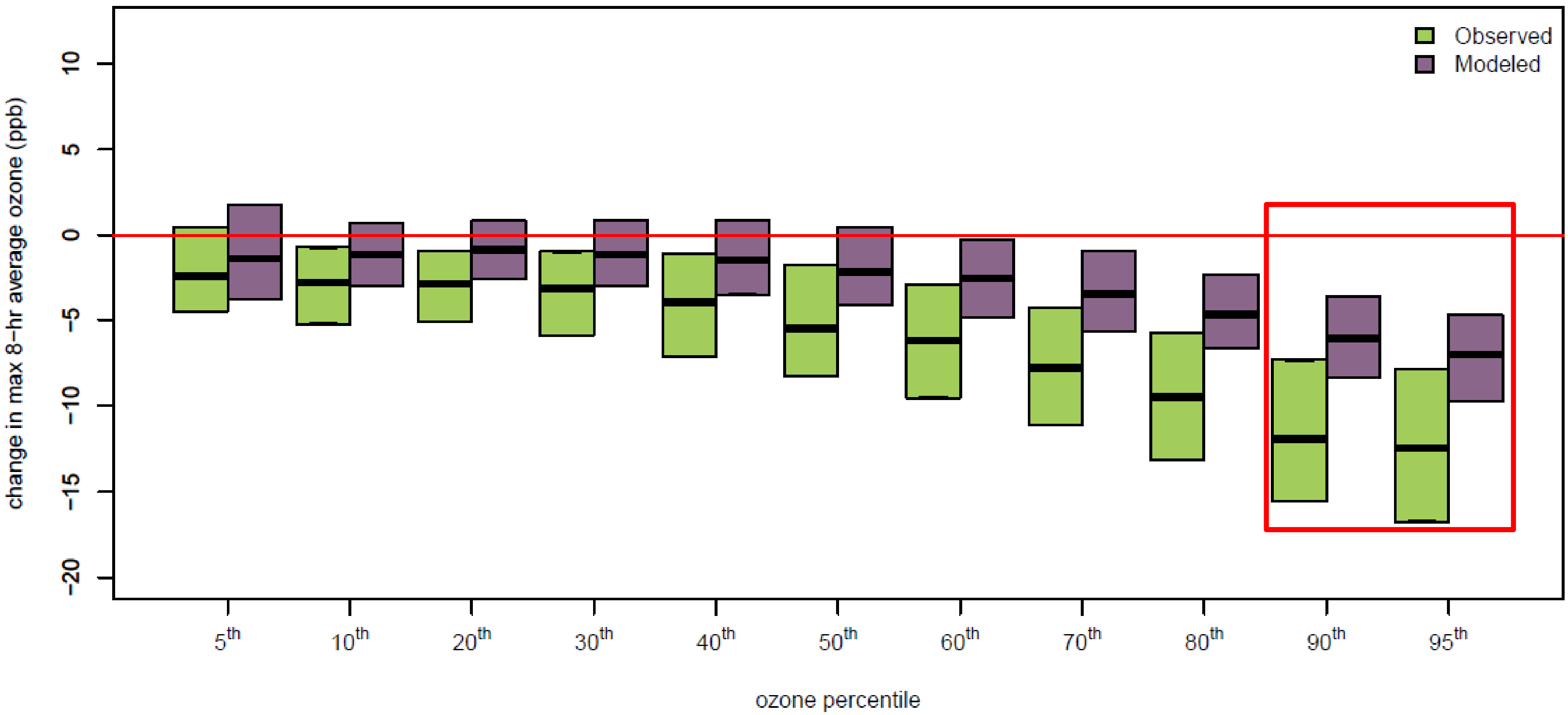
\+



=

2005 – 2002 total change in high summer ozone

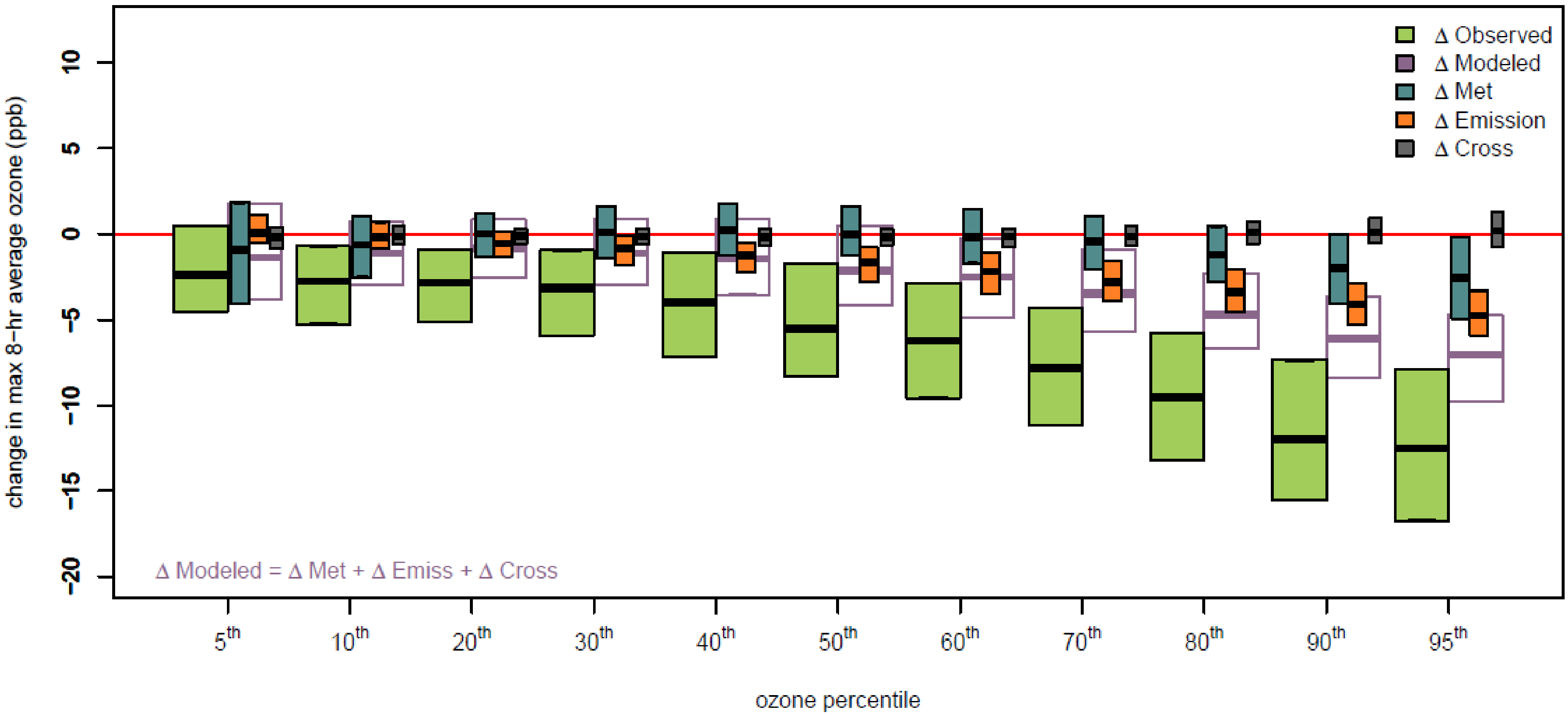
2005 – 2002 Change in Max 8hr Average Ozone by Percentile (ppb)



Each boxplot shows the distribution **across space** of the change in ozone at a certain percentile. (i.e. one value for each AQS site within NOx SIP Call states; n=444).

foley.kristen@epa.gov

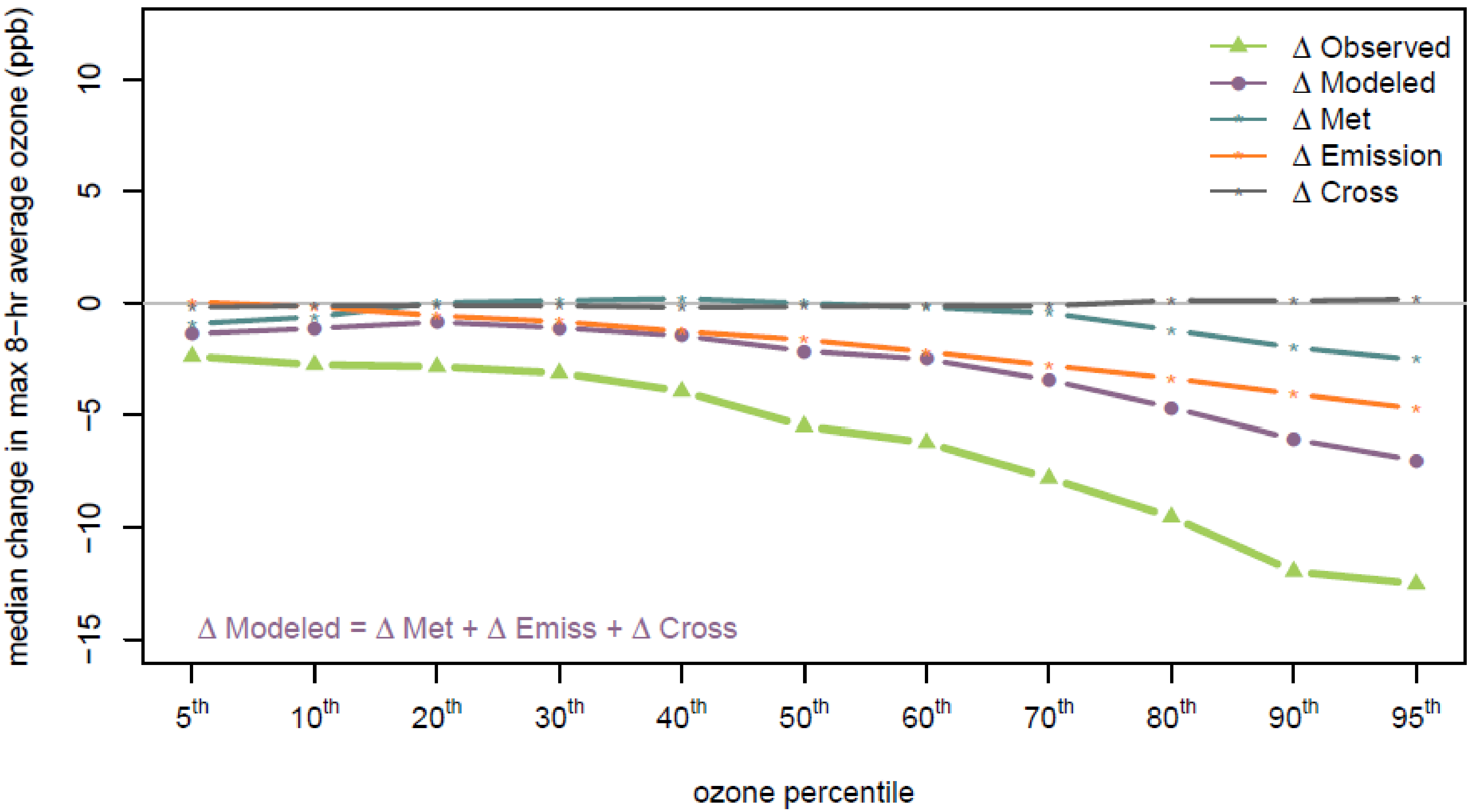
2005 – 2002 Change in Max 8hr Average Ozone by Percentile (ppb)



The change in ozone at each percentile can be decomposed into the change due to emissions, meteorology and the interaction between emissions and meteorology.

foley.kristen@epa.gov

2005 – 2002 Change in Max 8hr Average Ozone by Percentile (ppb)



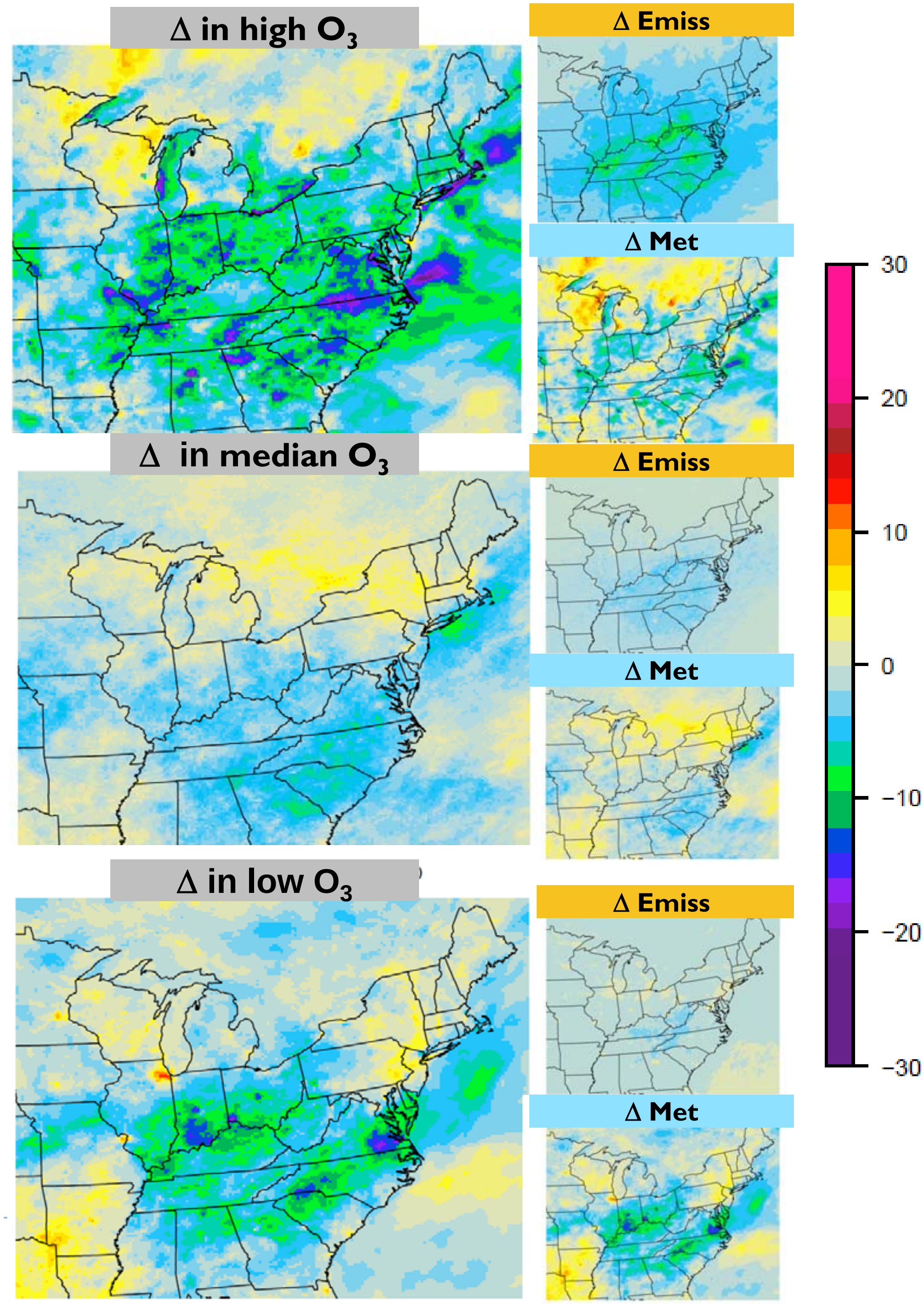
foley.kristen@epa.gov

Decomposing change in max 8hr average ozone

- Changes in the upper end of the ozone distribution are driven by both emissions and meteorology.
- The change in the lower end of the ozone distribution is driven almost entirely by meteorology changes.

In progress:

- Decompose change in NO_x and CO and compare meteorology-based changes to what we see in ozone.
- Evaluate predicted change in meteorological parameters (temp, winds speed, solar radiation) during "high" and "low" ozone days.

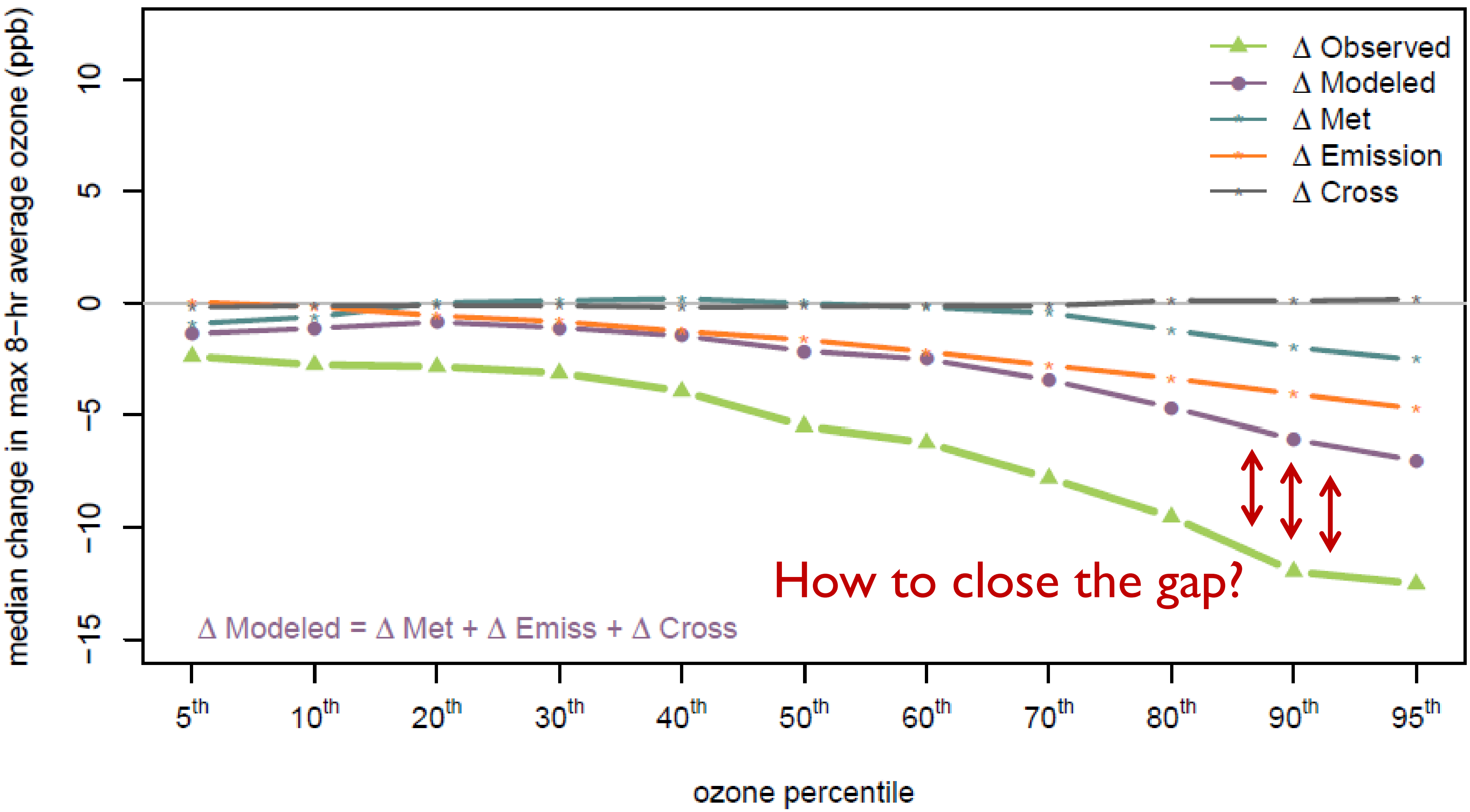


Conclusions

- Modeled change in ozone levels from 2002 to 2005 continues to be underestimated compared to observations in CMAQv5.
- Evaluation of NO_2 observations suggest emission inputs may underestimate the decrease in surface NO_2 emissions across these years.
- Decomposition of the change in summertime ozone shows the change in the upper end of the ozone distribution explained by emissions is similar in magnitude to the change in ozone due to changes in meteorology.
- Interaction between emissions and meteorology changes in this application is very small.

foley.kristen@epa.gov

2005 – 2002 Change in Max 8hr Average Ozone by Percentile (ppb)



foley.kristen@epa.gov

United States Environmental Protection Agency

Thank you for your attention!

Contact: Foley.Kristen@epa.gov