Evaluation of NOx Emissions and Modeling

Presenter: Barron Henderson

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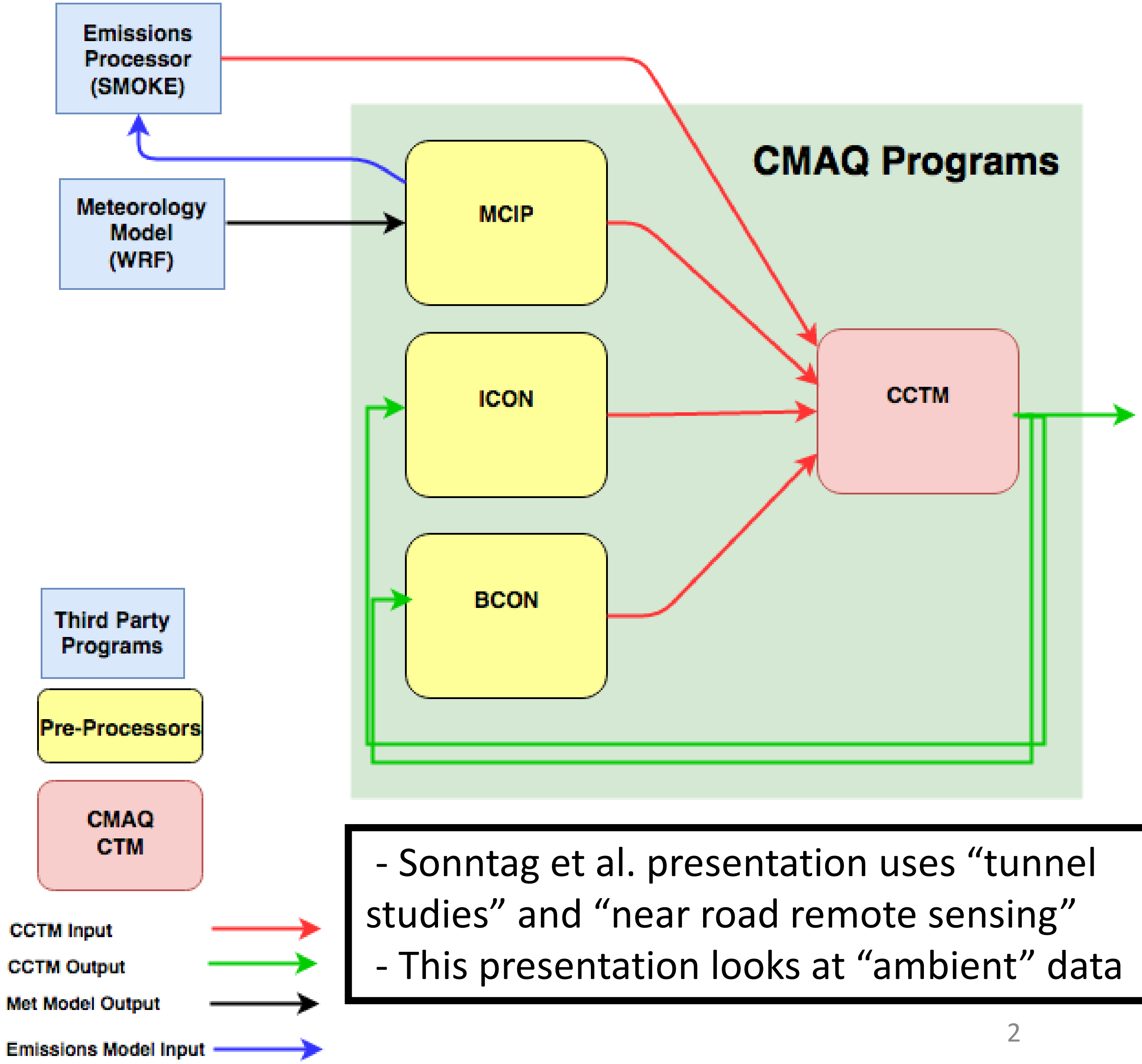
US EPA: Office of Air Quality Planning and Standards in collaboration with the Office of Transportation and Air Quality

Why do we inventory emissions?

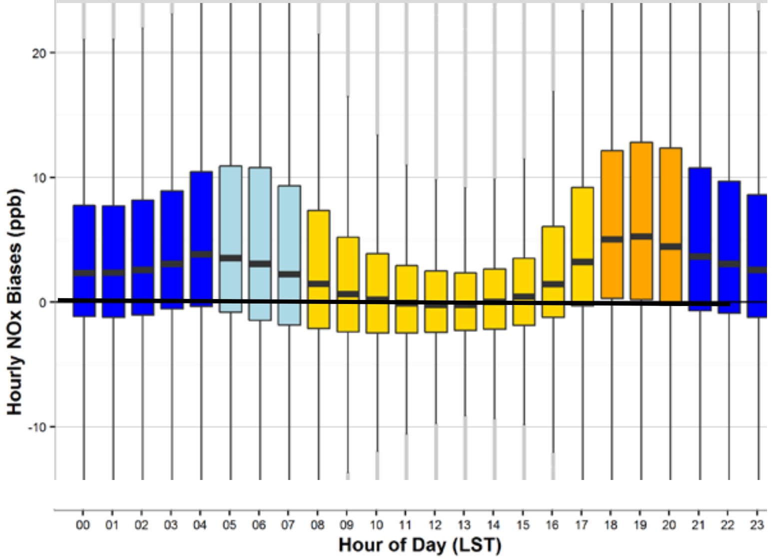
- Because they cause exposure
- We estimate exposure fields with monitors and models.
- Photochemical models
  - Community Multiscale Air Quality
  - Comprehensive Air quality Model with extensions
- What does it mean if modeled concentrations are higher than observed?
  - Emissions?
  - Physics/Chemistry?
  - Numerical solutions?



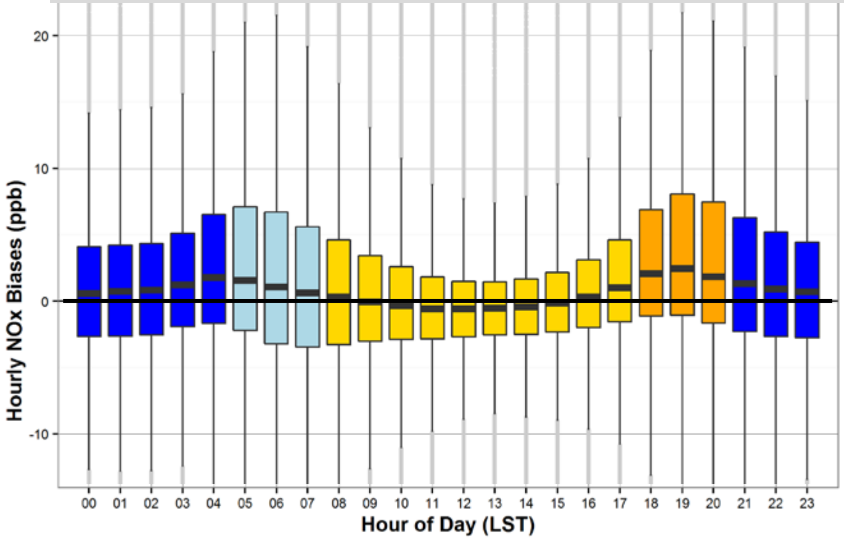
- Sonntag et al. presentation uses "tunnel studies" and "near road remote sensing"
- This presentation looks at "ambient" data

Past, Present, and... Future?

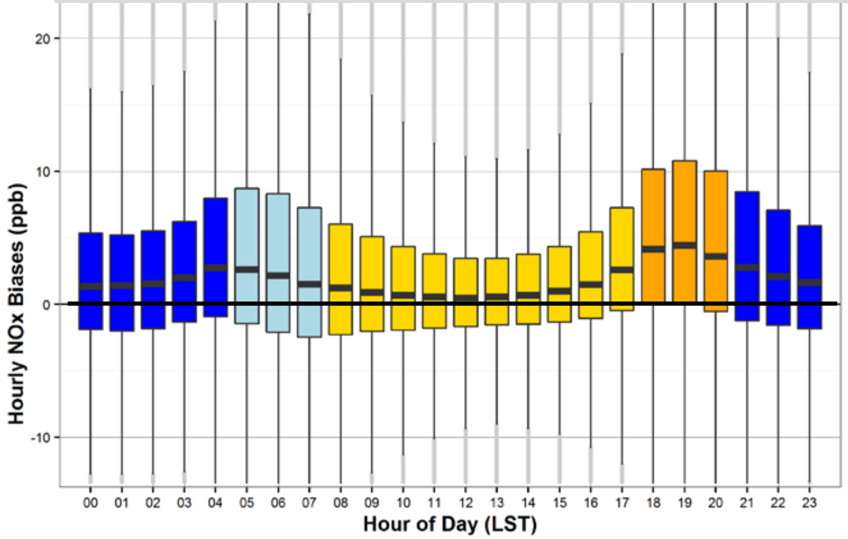
CMAQv5.0.2
NOx bias – all AQS sites



CMAQv5.1
NOx bias – all AQS sites



CAMx v5.2
NOx bias – all AQS sites



- NOx is generally **unbiased** or **under-predicted** during daytime but is **over-predicted** in morning and **evening** transition hours and at **night**
- CMAQv5.1 has improved characterization of mixing in morning/evening transitions and at night compared to CMAQv5.0.2
  - NOx biases decrease in CMAQv5.1 versus CMAQv5.0.2
- CAMx v6.2 biases in NOx generally fall between biases from CMAQv5.0.2 and v5.1
- While we previously evaluated NO_y bias against AQS measurements, after further evaluation, we not longer believe that AQS NOy measurements are accurate enough/appropriate for that purpose

Recent community developments

- Anderson et al (2017) cited as mobile 2x over prediction.

- Travis et al (2017) published “Why do models overestimate surface ozone in the Southeast United States?”
  - D. Jacob (Harvard) group along with NOAA/NASA coauthors
  - Uses a sensitivity where all non-EGU emissions cut by 50% and shows less bias
  - Already being frequently cited in the literature

Coordinated efforts within the agency and across agencies

- Technical discussions on Emissions and Atmospheric Modeling (TEAM)
  - Cross-agency coordination
  - Point of contact: Barron Henderson, Greg Frost (NOAA) and Barry Lefer (NASA)
  - 3 Webinars have been held
  - Upcoming session at the American Geophysical Union (AGU) conference in New Orleans in Dec 2017
- Cross-Office NOx Evaluation Work (COEW… not using acronym)
  - OAQPS, OTAQ, ORD
  - Diverse perspectives, committed to continual improvement
  - Targeting research to address community questions.

High priority hypotheses

Model bias caused by mismatch of modeling grid-cell average compared to measurement location
Model bias caused by issues related to vertical mixing
Dry deposition velocities for NOy species are too low in models
Model bias is due to some unique feature of summer 2011 platform
Onroad emissions rates are too high
MOVES default inputs inflate emissions
Nonroad emission rates are too high
National nonroad equipment population/activity is overestimated
HD running emissions are at the wrong time of day
Onroad HD temporal profiles allocate too much of the emissions to rush-hour time periods
Non-CEMS EGU emissions are inappropriately allocated from annual to hourly emissions
Monthly, day-of-week, and/or diurnal temporal profiles for nonroad equipment are incorrect
Spatial allocations (county to grid cell) are incorrect for onroad emissions
Spatial allocation (county to grid cell) of nonroad equipment is incorrect.
Spatial allocation onroad activity by MOVES from national to county-level
Nonroad emissions spatial distribution (national to county) is wrong

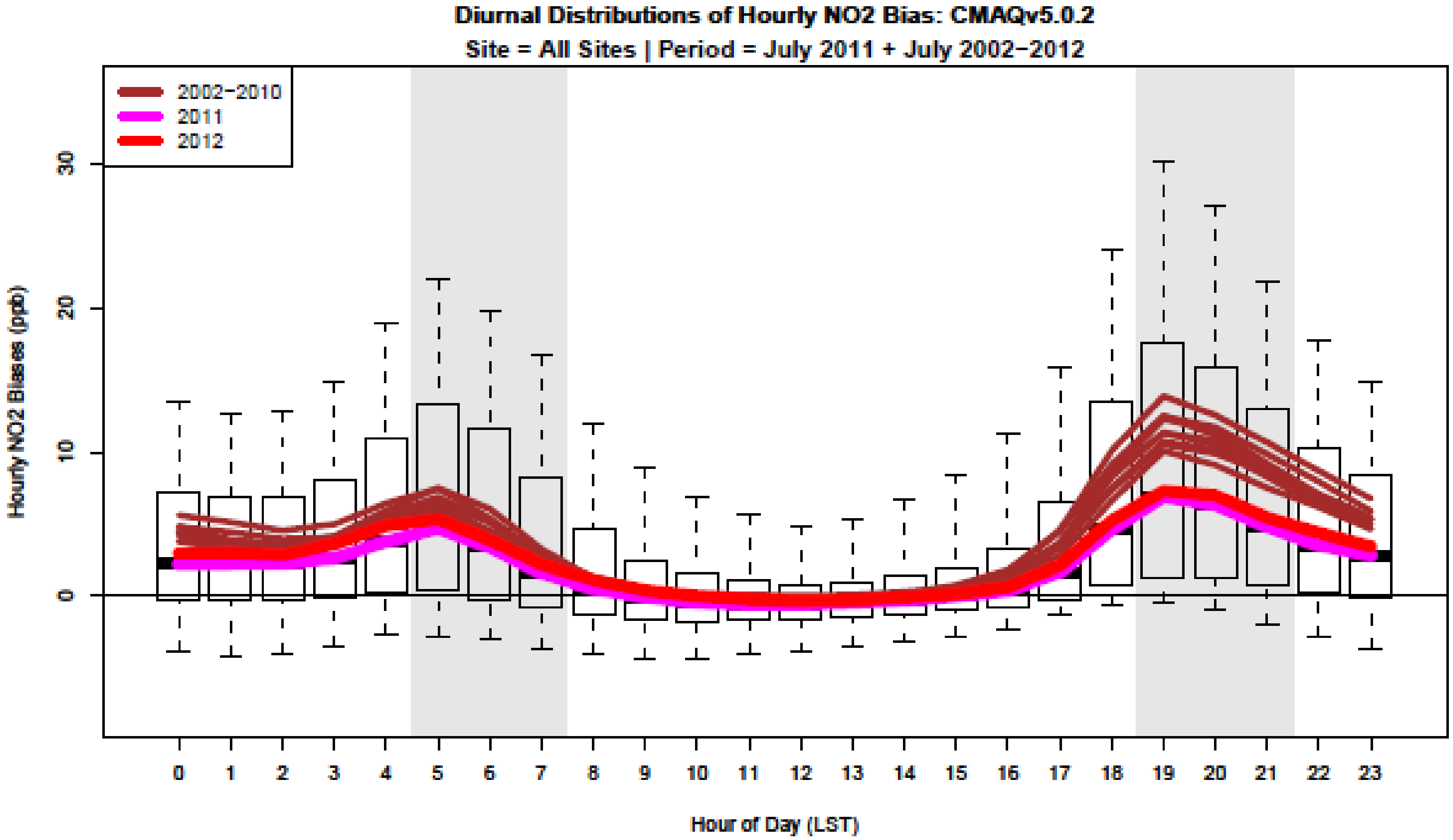
A Lot of Ideas; too much text!

Overview of Today's Presentation

Hypothesis
Model bias is due to some unique feature of summer 2011 platform
HD running emissions may be allocated to the wrong time of day.
Vertical mixing is under predicted causing high bias in NOx
Nonroad equipment emissions are over estimated or misallocated temporally
Non-CEMS EGU temporal misallocation from annual to hourly emissions
MOVES default inputs inflate emissions
Methods for estimating NOx Emissions bias are biased

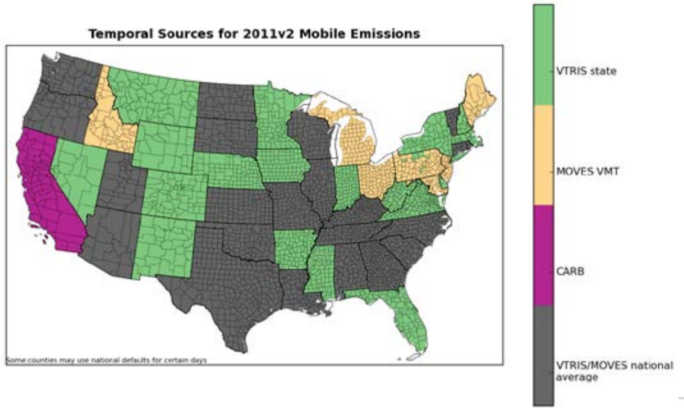
Hypothesis: Model bias is due to some unique feature of summer 2011 platform

- Using 2002 – 2012 time series of CMAQv5.0.2 simulations, NO_2 bias at 250 AQS sites across the country is less in 2011 than in other years



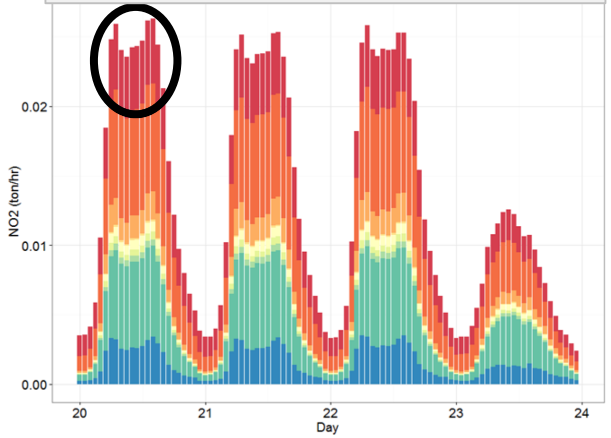
Foley ORD lead

Hypotheses: HD running emissions may be allocated to the wrong time of day.

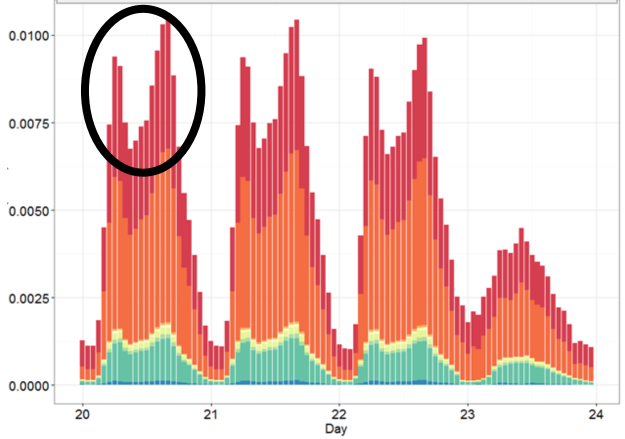


- **Background:** EPA developed new national default hour of day profiles for LD cars/trucks and HD diesel trucks that were incorporated into the 2011 modeling platform

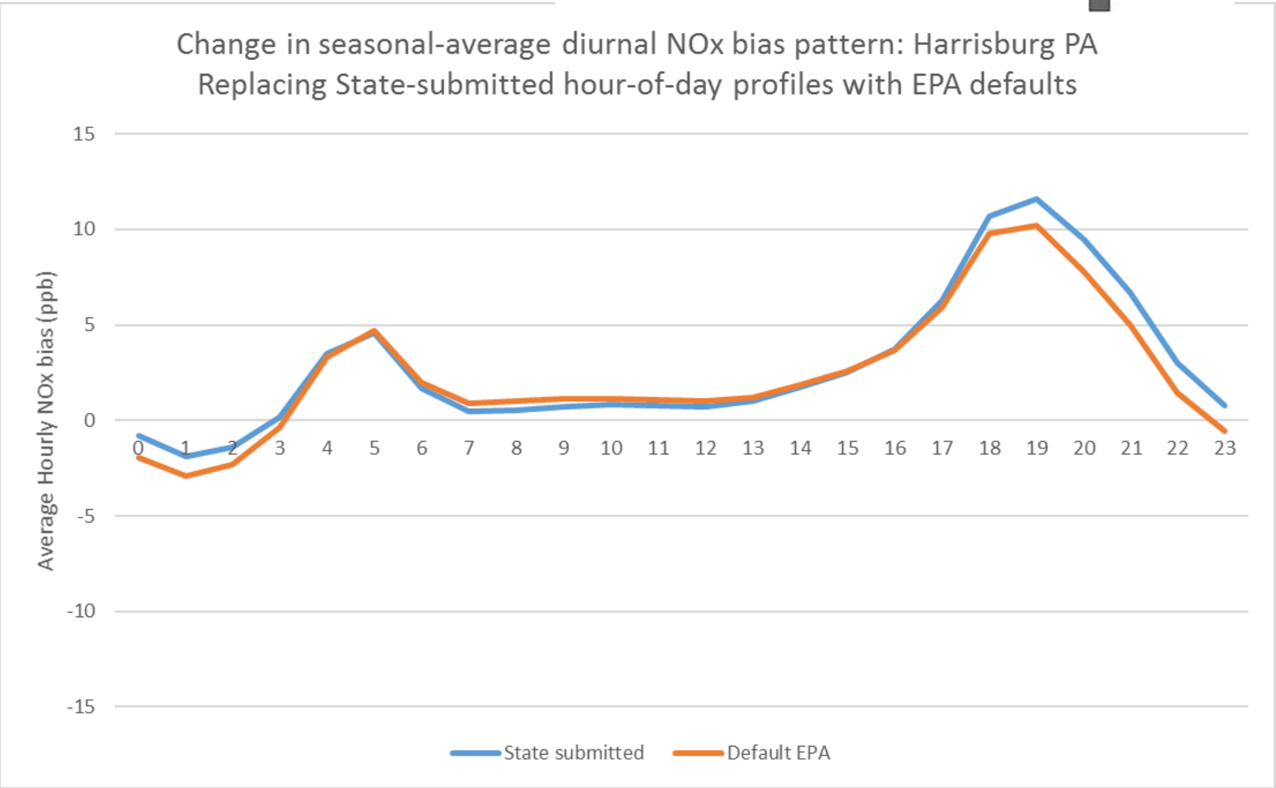
NO_2 emissions from HD sources DC, July 2011.



NO_2 emissions from HD sources Beltsville, MD, July 2011.



- **Sensitivity:** Re-run CAMx for summer 2011 using national default hourly profiles for on-road LD and HD emissions.
- **Results:** Change tends to slightly dampen "bridge pattern" in diurnal NOx/NOy biases (reducing overestimates at night), but changes small from a national perspective.

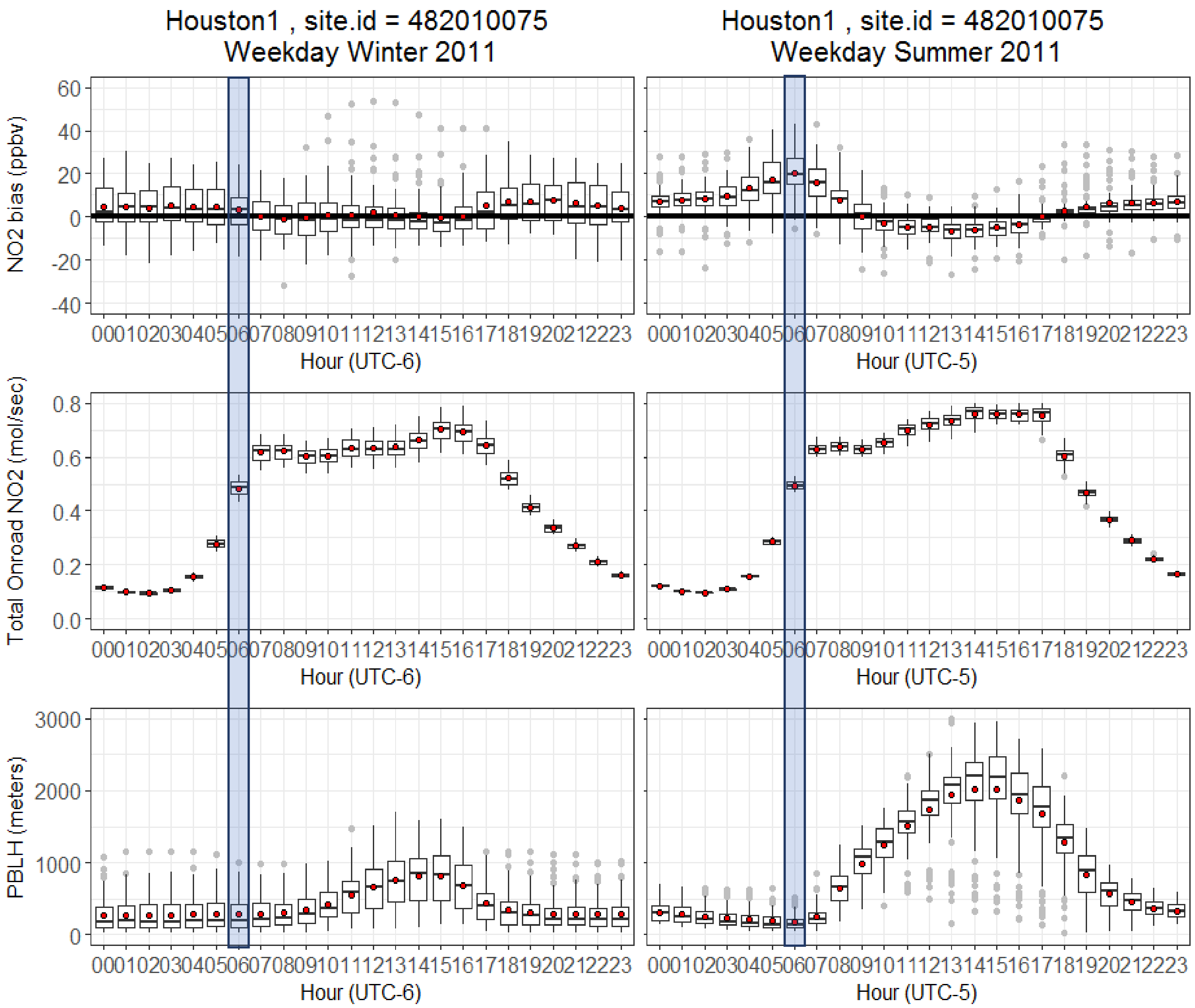


Harrisburg PA shows the largest NOx bias improvement of any site.

Toro, Eyth, and Dolwick leads

Hypotheses: Vertical mixing is under predicted causing high bias in NOx

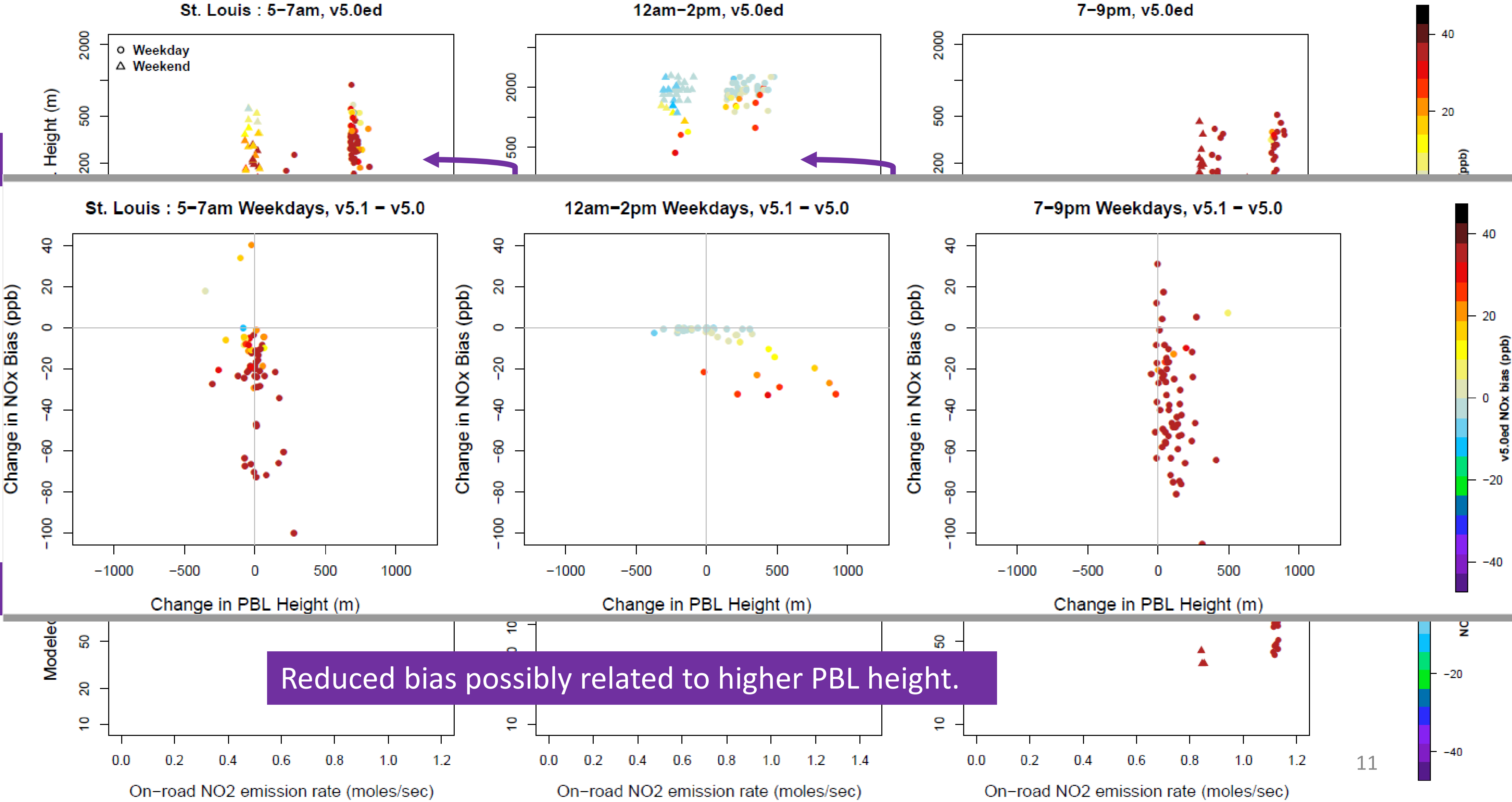
- Distinct seasonal patterns in NO2 bias: prominent summertime morning bias is absent in wintertime comparisons
    - Consistent with previous EPA evaluation of NOx bias
    - Modeled morning NO2 concentrations did not change much between seasons while observed morning NO2 was much lower in the summer
    - Onroad mobile NO2 emissions during morning hours were similar in summer and winter
    - Nonroad mobile NO2 morning emissions were somewhat higher in summer than in winter
    - Model predicts morning PBL height is lower in summer than in winter
- Pending follow-up items
    - NONROAD sensitivity simulations
    - Further analysis of PBL and LSM schemes in CMAQ



Toro *lead*

Hypotheses: Vertical mixing is under predicted causing high bias in NOx

CMAQv5.0



CMAQv5.1

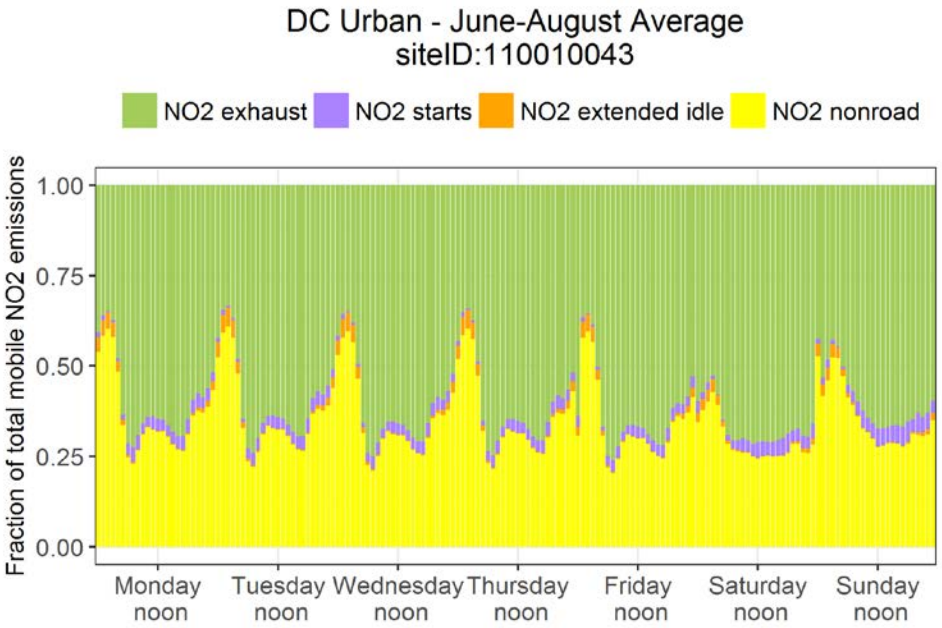
Reduced bias possibly related to higher PBL height.

Foley *lead*

Hypotheses: Nonroad equipment emissions are over estimated or misallocated temporally

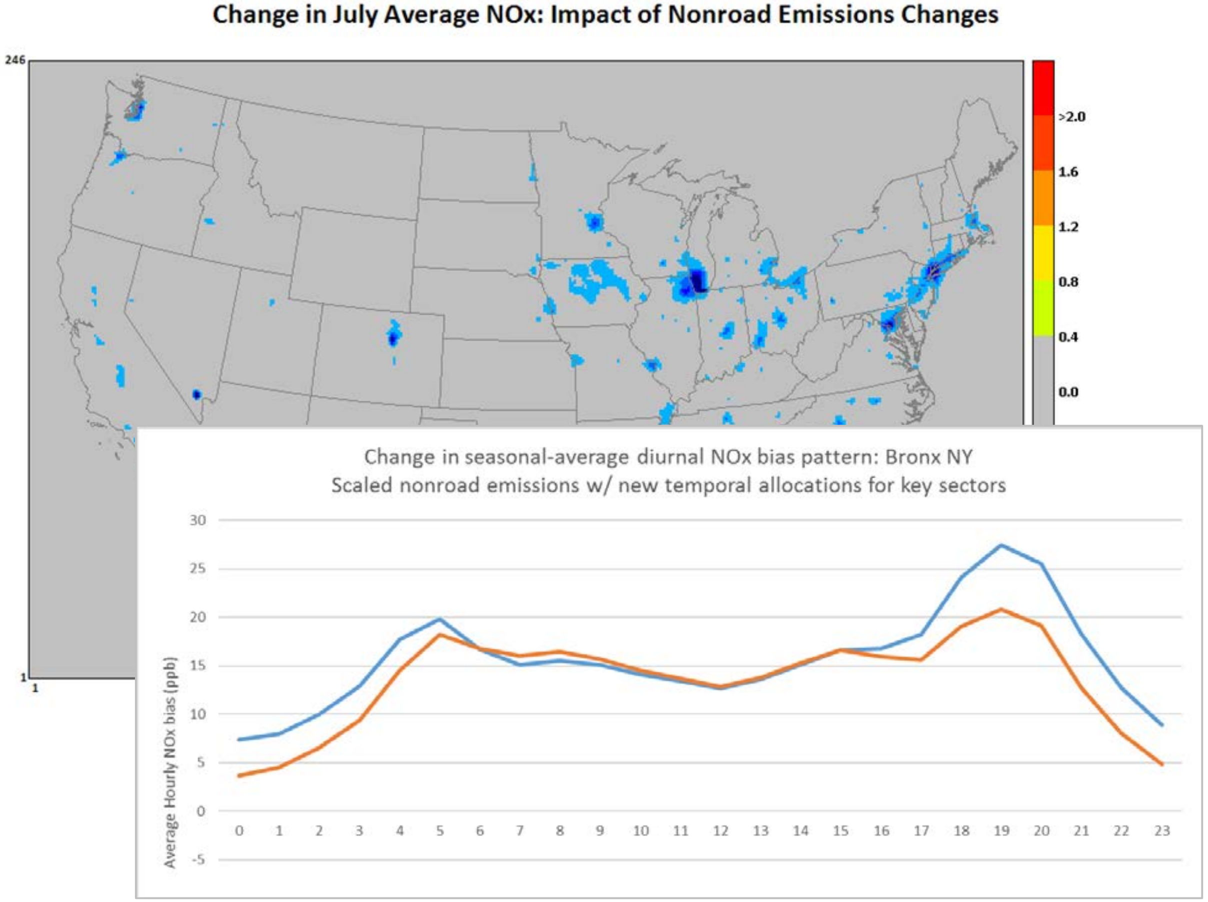
- Identified issues with existing temporal profiles for Construction, Lawn & Garden, and agriculture emissions: WD/WE and day/night allocation.

- Using interim national scaling factors, a national reduction of nonroad NOx emissions of ~ 7% is obtained for 2011.



Results:

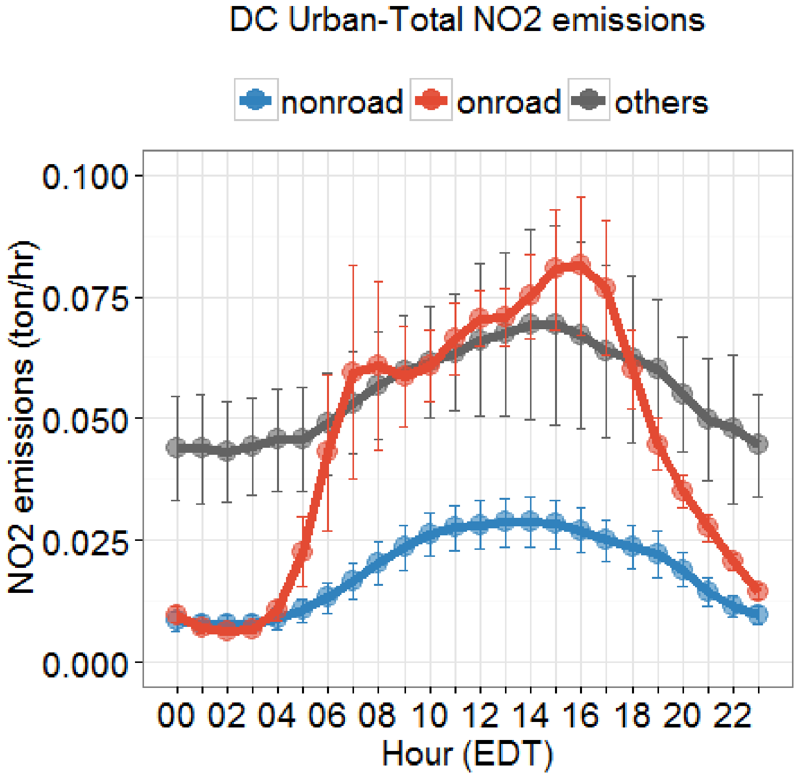
- Although a small decrease in NOx national average, the change impacts NOx bias during non-daytime hours.

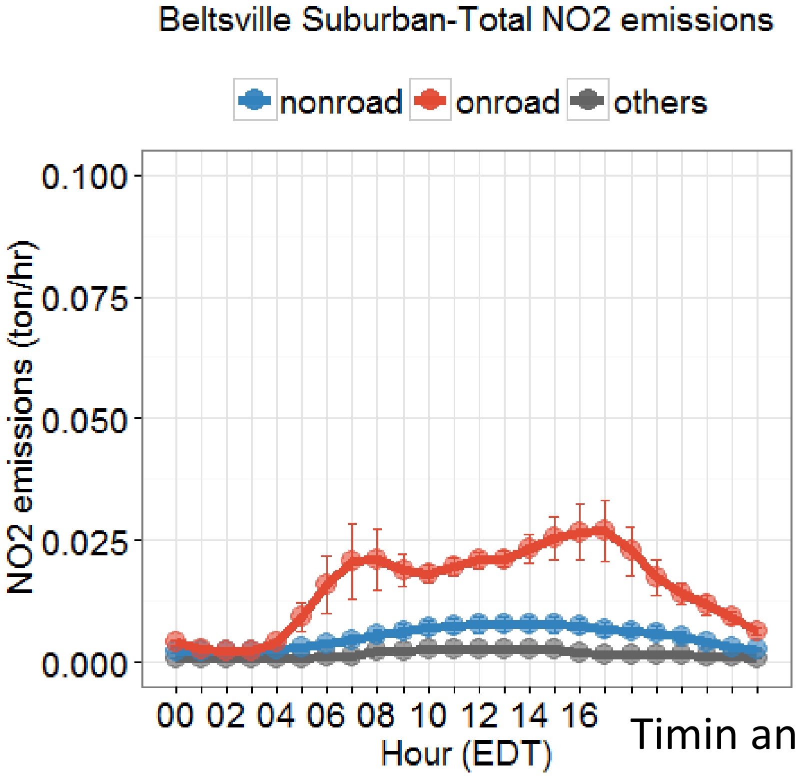


OAQPS (Timin, Dolwick) and OTAQ (Toro, Roberts) collaboration

Hypothesis: Non-CEMS EGU temporal misallocation from annual to hourly emissions (1/2)

- Emissions from EGU are similar in magnitude (and larger at nighttime) than onroad mobile emissions during period studied
- Source apportionment analysis suggest EGU emissions are significant predictor of NOx bias



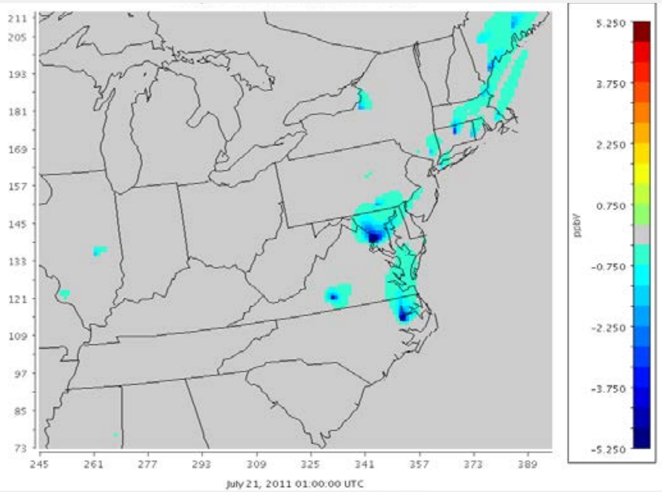


Timin and Dolwick *leads*

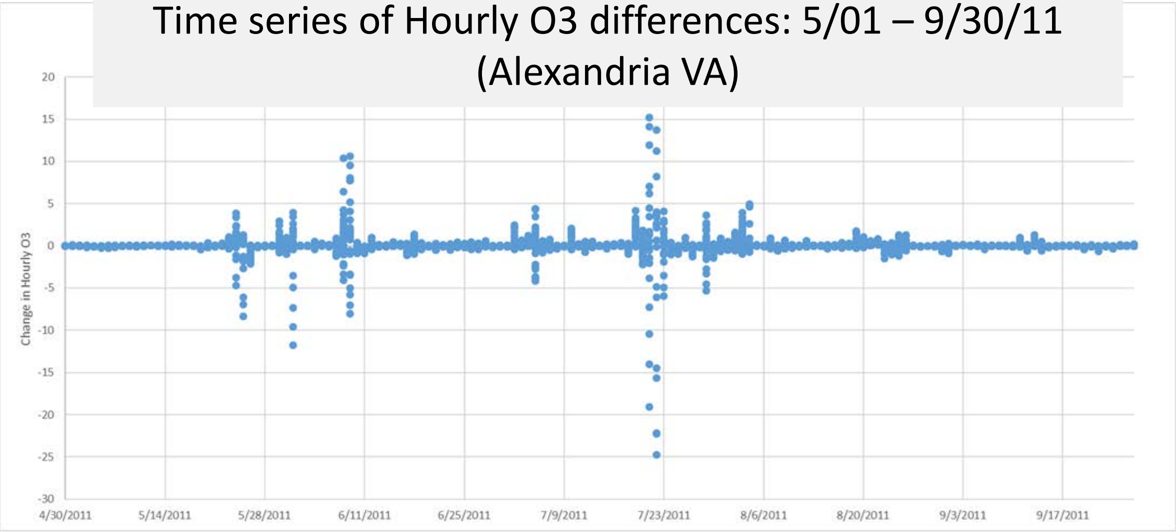
Hypothesis: Non-CEMS EGU temporal misallocation from annual to hourly emissions (2/2)

- **Background:** There are ~57,000 TPY of NOx in 2011 at non-gas, non-coal sources that are in the EGU modeling sector, but do not have hourly CEMS data.
  - The annual emissions from these sources are temporalized based on an approach that has been found to be inappropriate for many of the sources (e.g., municipal waste combustors, paper mills, etc.).
  - The original temporalization was based on a regional average temporal profile which looks like an EGU peaking unit. In reality, the municipal waste combustor and cogeneration units likely operate everyday on a fairly regular schedule.
- **Sensitivity:** Re-run CAMx for summer 2011 using a flat (or nearly flat) temporal profile for all non-CEMS sources that are in the EGU sector.
- **Results:** Very small changes in O3, NOx, NOy on most days over the U.S. By far, the largest impacts were detected in the MD/DC/VA region on July 21st and 22nd. As a result, care should be exercised when looking at pre-fix EGU impacts.

Sample Hourly NOy differences: July 21, 2017



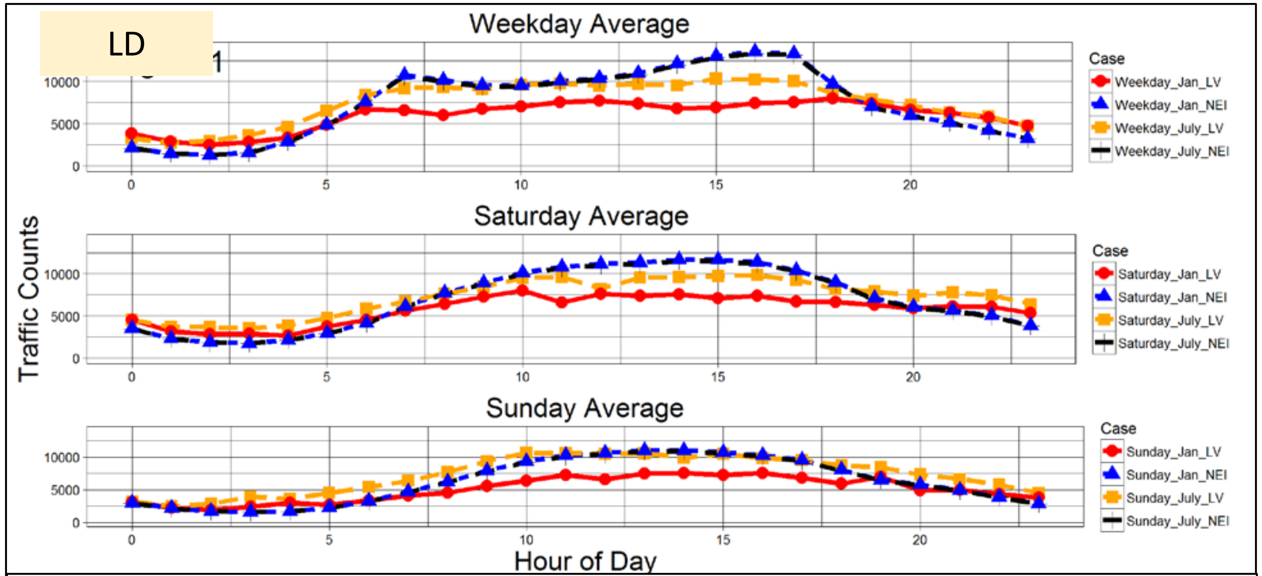
Time series of Hourly O3 differences: 5/01 – 9/30/11 (Alexandria VA)

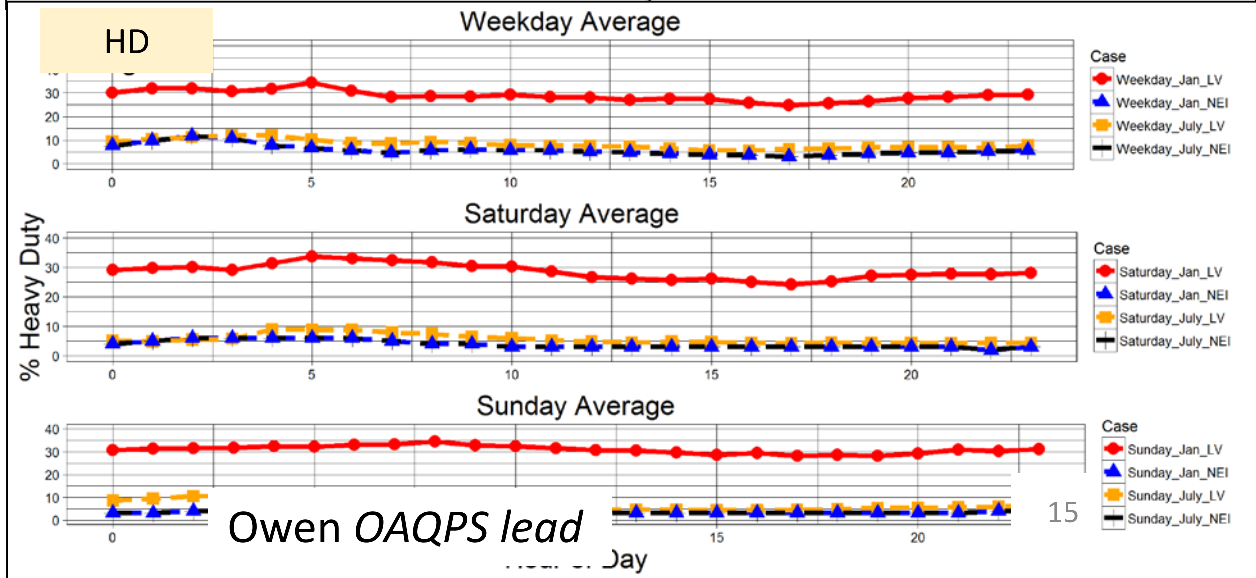


Timin and Dolwick *leads*

Hypotheses: 1) Onroad emissions rates too high; 2) MOVES default inputs inflate emissions.

- Las Vegas near-road measurement campaign was conducted in 2009 along I-15 in Las Vegas
  - In cooperation with FHWA, EPA is applying this data to evaluate MOVES inputs and emissions for this location
  - Traffic patterns – As a first step in evaluating these platforms, we compare traffic counts from the field study to those used in the EPA's 2011 modeling platform, focusing on diurnal and weekday and weekend traffic activity and total highway running exhaust emission rates from the on-road sector.
- Light duty traffic
  - Traffic counts for NEI are fairly similar on weekdays and weekends in both summer (July, black lines) and winter (January, blue lines)
  - January field data (red lines) shows much lower total traffic volumes versus July field data (orange lines) on all days
  - Field data indicates lower traffic volumes than NEI estimates, with a greater difference in January than July
  - Field data do not show the morning and afternoon peaks indicated in the NEI estimates and the timing of traffic increases start earlier in the field data
- Heavy duty traffic
  - Percentage of heavy-duty vehicles are fairly similar between NEI cases and the July field data, though January field data shows much higher percentages.
  - Differences in heavy-duty distribution in January and total volumes could be issue with traffic data or due to the onset of the financial recession early 2009.
  - The observed traffic data likely reflect I-15 construction and lane closures that occurred in 2009

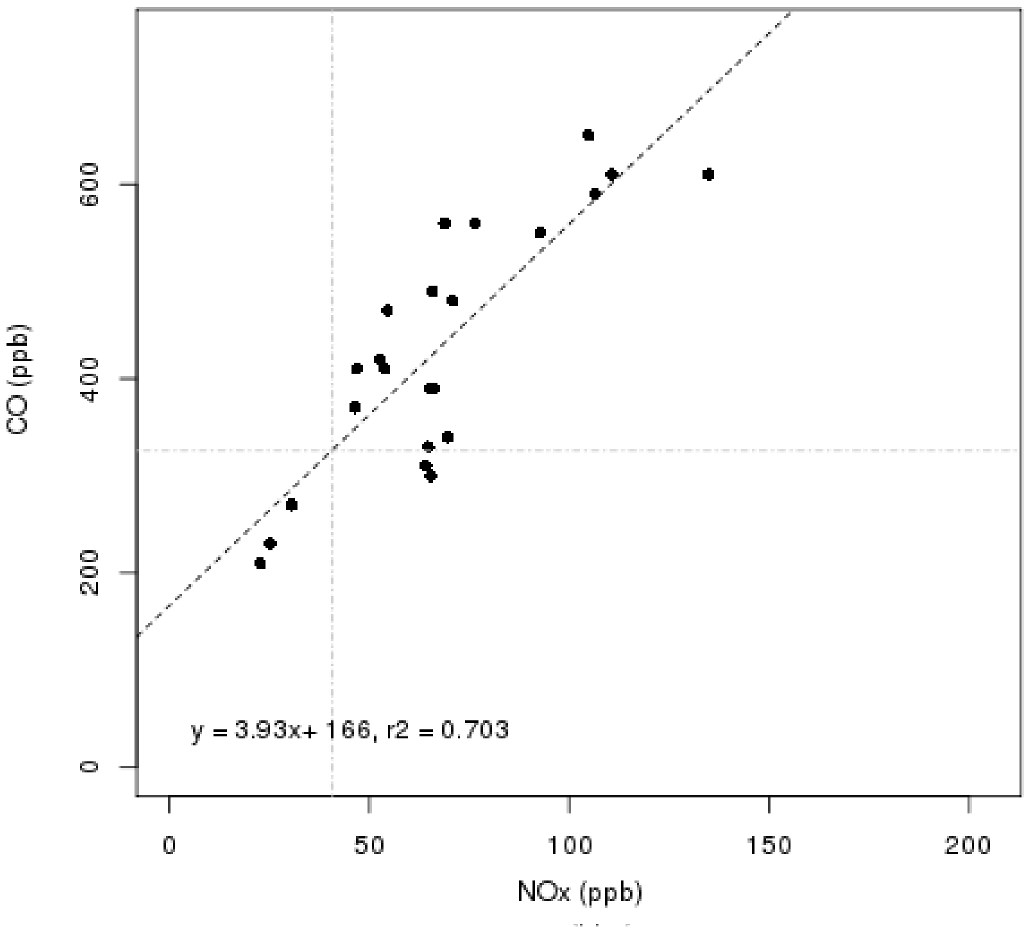




Owen *OAQPS lead*

Hypothesis: Methods for estimating NOx Emissions bias are *biased*

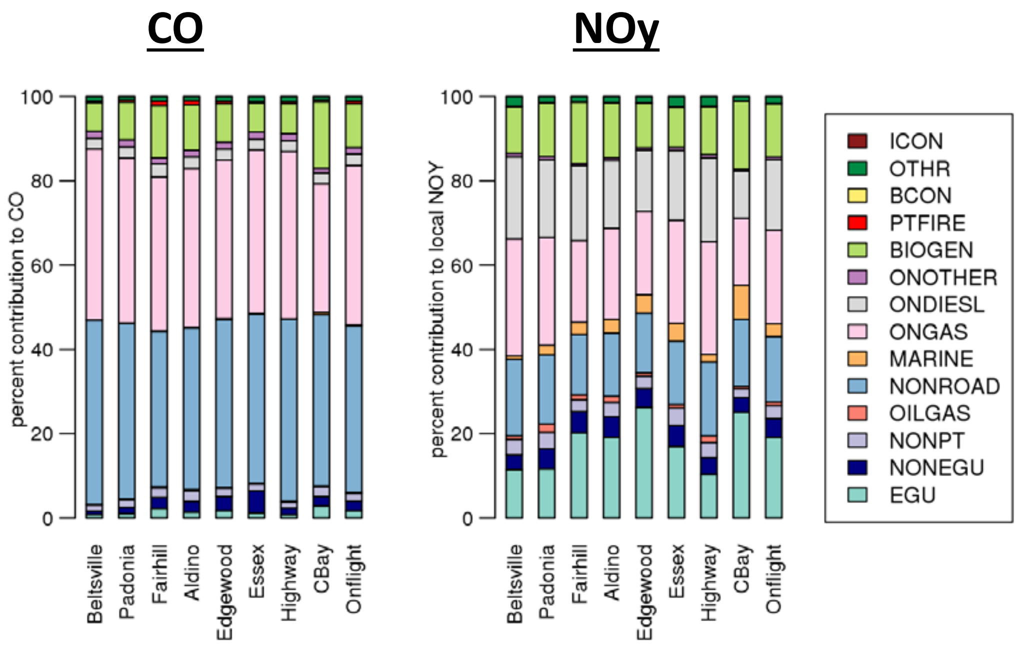
- Background: Relationships between CO and NOy have been used evaluate inventories
  - The slope of CO vs NOy is commonly derived from linear regressions *y = mx + b*
    - *y* = CO; *x* = NOy
    - *m* = ΔCO:ΔNOy; *b*=CO(bkg)
  - CO acts as a tracer and therefore is assumed to normalize for any uncertainties in mixing
  - The slope (slope = ΔCO:ΔNOy) represents the increment above "background" which researchers argue can be compared directly to local emissions ratios
  - e.g., Anderson et al (2014) concludes mobile E(NOx) over-estimated mobile emissions by 2x for DISCOVER-AQ campaign
- We conducted source apportionment modeling to answer questions about
  - Reasonability of bias attribution to onroad sector
  - Photochemical aging of emissions ratio.
  - Influence of measurement uncertainty



Simon et al. *internal review*

Bias should not be attributed only to onroad NOx

- Top 3 sources of CO include: nonroad, onroad gasoline, and biogenic
- Important sources of NOy include: EGUs, nonroad, biogenic, onroad gasoline and onroad diesel



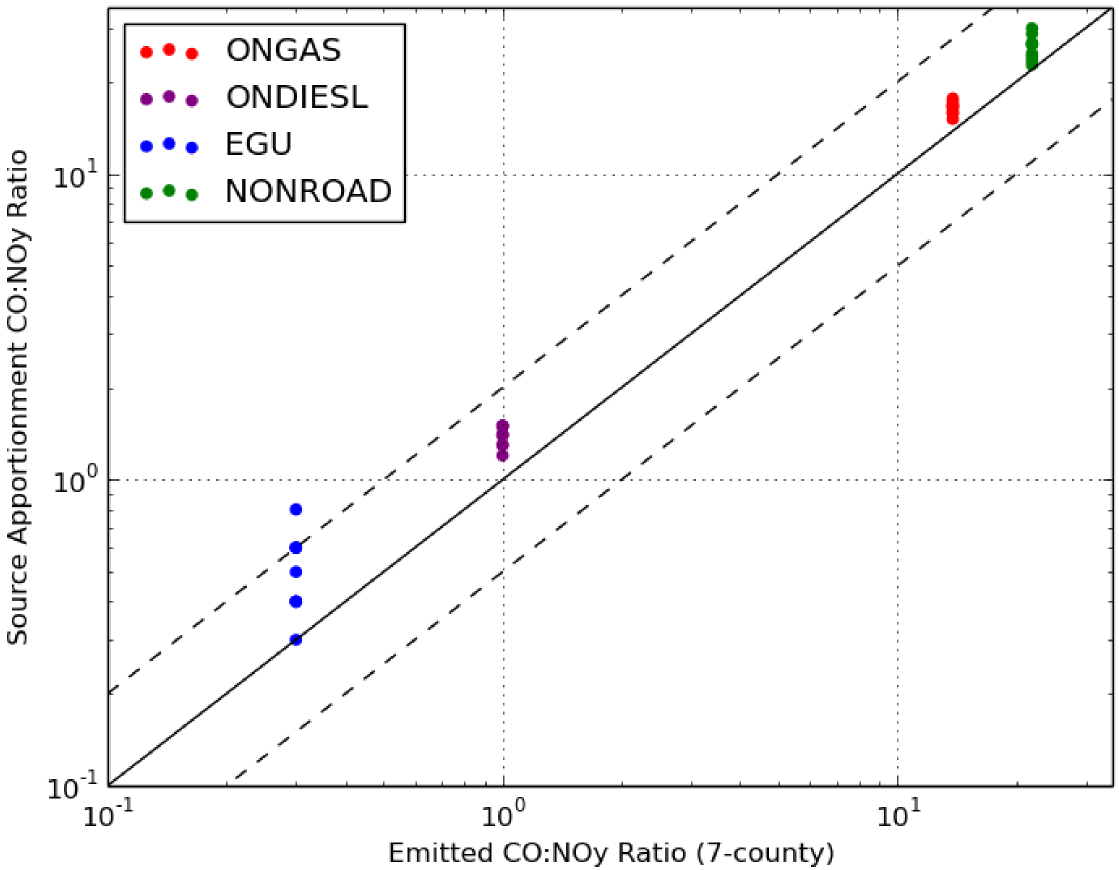
Tag	Emitted CO:NOx
EGU	0.3
NONEGU	11.5
NONPT	2.9
OILGAS	0.9
NONROAD	21.9
ONGAS	13.8
ONDIESL	1.0
ONOTHR	20.7
MARINE	0.1
PTFIRE	102.3
OTHR	44.7

- Emitted CO:NOy ratios from these source vary by several orders of magnitude (0.1-20)
- Attribution inferred from good point source assumption, ignores NONROAD and aging.

Simon et al. *internal review*

Aging significantly affects slopes post-emission

- Using source apportionment allows us to track CO:NOy as a function of source.
- Sector Concentrations by site
  - Sites: Aldino, Beltsville, Chesapeake Bay, Edgewood, Essex, Fairhill, Highway, Onflight, and Padonia
  - Sectors: On-road gasoline, on-road diesel, EGU, and Non-road
- Emissions averaged for the 7-county area; assumes low variability from site-to-site in emissions (similar to Anderson 2014 Fig 4)
  - EGU and NONROAD emitted ratios actual vary a lot
  - On-road gasoline do not
- 5-50% of bias is attributable to aging within sector
- Ignores cross-sector net-aging



Concentration ratios as a function of emitted ratios

Simon et al. *internal review*

Not all NOy is equal: observations and models

- CO:NOy slopes:
  - Ordinary Least Squares
  - Measurements: Total NOy and Sum of NOy(i)
  - Model: Sum of NOy(i)
- Total and Sum of NOy slopes
  - 1/3 of regressed measurements are statistically inconsistent (slope CI95% non-overlapping).
  - Filtered where regressions by both measurements agree.
- Modeled ΔCO:ΔNOy slopes
  - Are not rejected by t-test except over highway location
  - Day-to-day variability was much lower

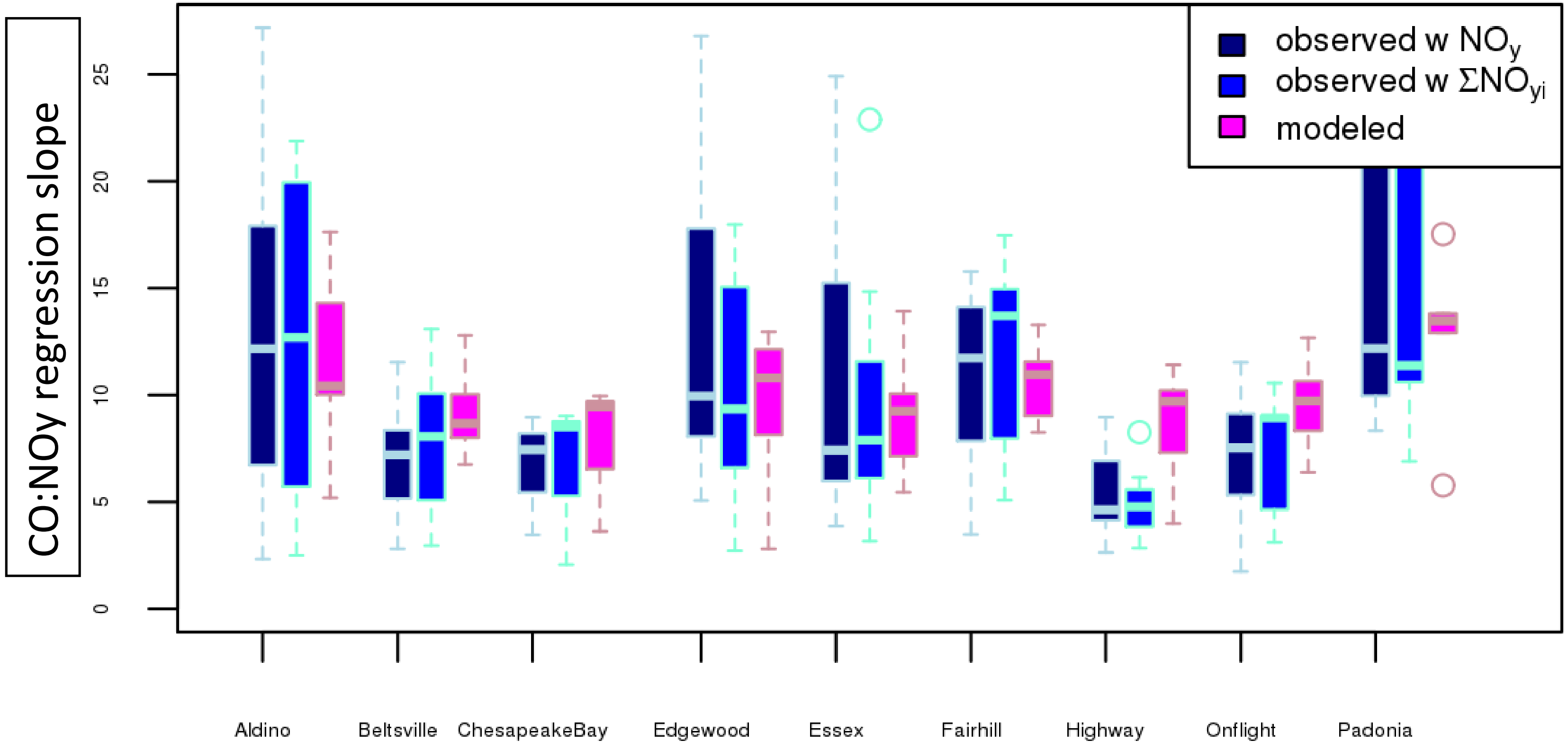


Figure shows comparison of modeled and measured ΔCO:ΔNOy for days/locations with statistically significant regression slopes

Simon et al. *internal review*

Next Steps

- Continue ongoing analyses at EPA
  - Hypothesis table will continue to serve as a guide for prioritizing efforts
- Step up engagement with outside community (conferences and TEAM) to further investigate this problem
  - Engage with field study designers within and outside EPA to encourage field study designs that can help answer specific questions on NOx emissions
- Synthesize EPA analysis to this point and determine if/what concrete updates can be made to emissions and modeling platforms (e.g. appropriate updates from CAMx sensitivity simulations and others)