Evaluating Updates to CAMx and NOx Emissions using TEMPO Measurements over Texas

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AQRP 24-004

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TEMPO instrument launch on board IntelSat 40e on April 7, 2023

Credit: Walter Scriptunas/Center for Astrophysics | Harvard & Smithsonian

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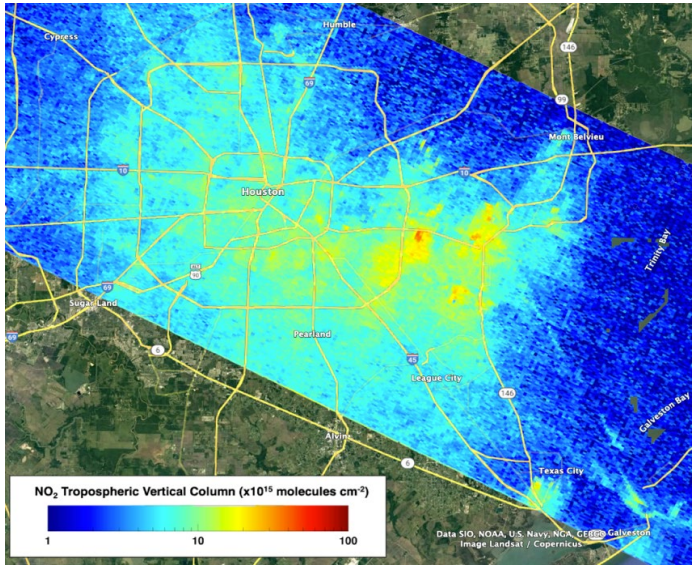
Motivation for Project 24-004

- Our previous AQRP project (22-023) showed that highly resolved NO_2 columns (250 m x 560 m) can constrain the Houston NOx emission inventory with source-category specificity
- TEMPO provides coarser spatial resolution (2.5 km x 5.0 km) than GCAS aircraft measurements, but TEMPO also provides hourly data resolution (cloud-free/daylight hours) over more days over much larger area
- **Goal**: Can NO_2 columns from the Tropospheric Emissions: Monitoring of Pollution (TEMPO) satellite can similarly constrain the Houston (and rest of East Texas!) NOx emission inventory with source-category specificity?
- Use 3-D CAMx tagged NO_2 to evaluate NOx EI against TEMPO NO_2

GCAS aircraft column NO_2 measurements from 5.3 mi (8.5 km) altitude



TEMPO column NO_2 measurements from 22,000 mi (36,000 km) altitude

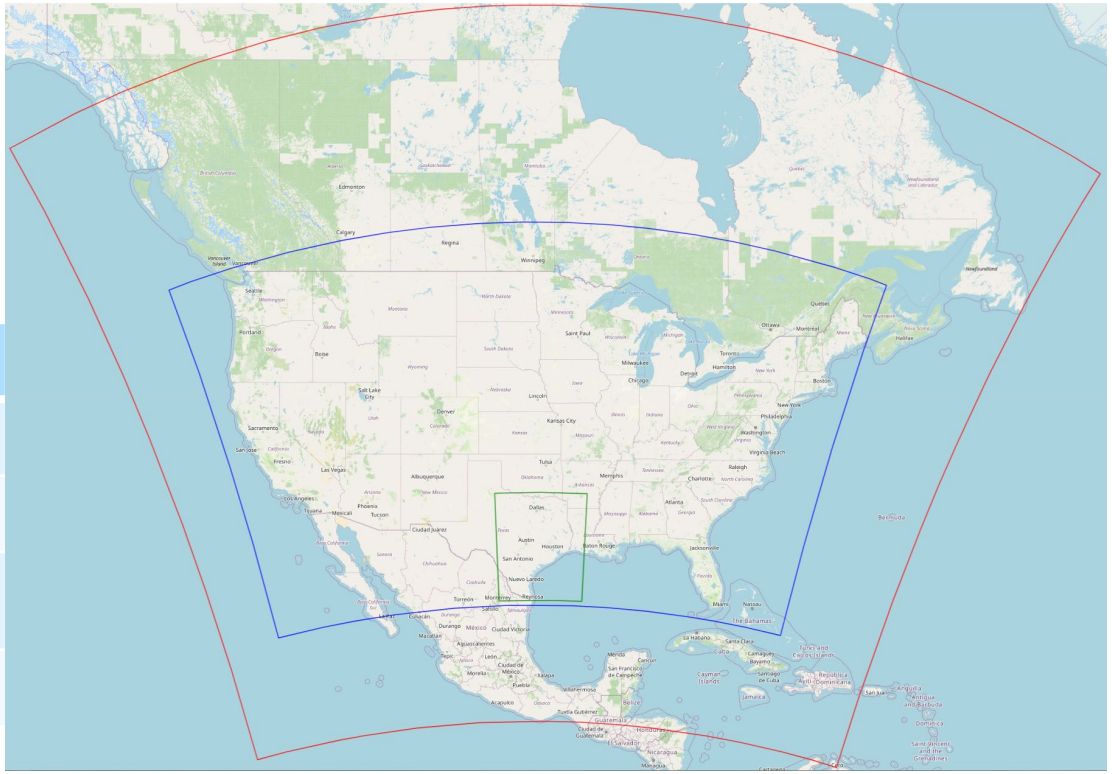
Source: NASA Worldview

GCAS: GEOstationary Coastal and Air Pollution Events Airborne Simulator

Baseline CAMx Configuration

- CAMx modeling episode: Aug 25-Sep 30, 2023
- Ramboll WRF run for TCEQ 36/12/4 km SIP domains
- Anthro emissions from TCEQ 2019 SIP (same as AQRP Houston GCAS)
- 3-D CAMx tagged NO_2 by sector

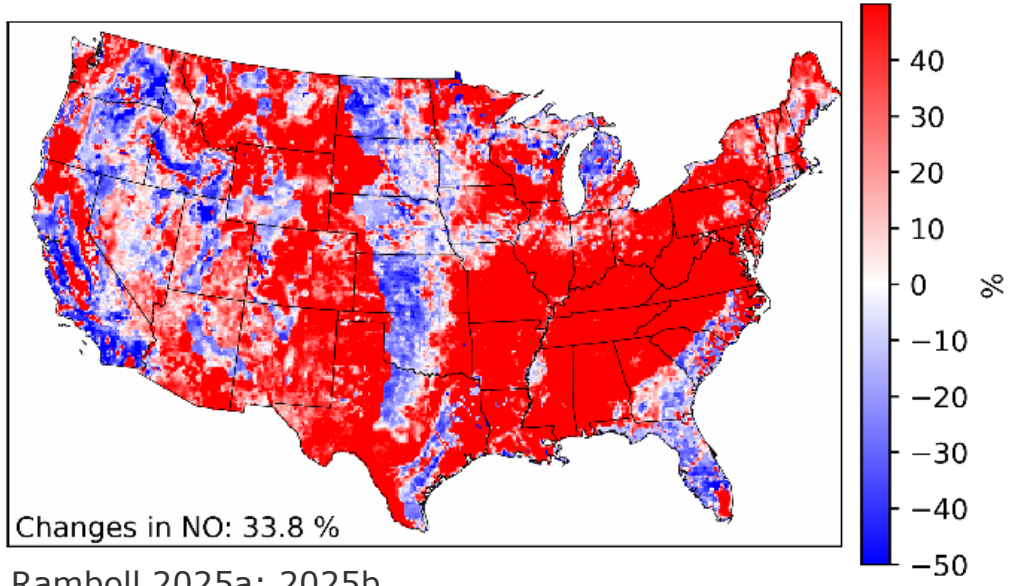
No.	Source Sector	No.	Source Sector
1	Biogenic (soil NOx)	5	Off-road mobile including shipping
2	Lightning NOx	6	Electric Generating Units (EGUs)
3	Aircraft climb-out and cruise	7	Oil and Gas
4	On-road mobile	8	Other



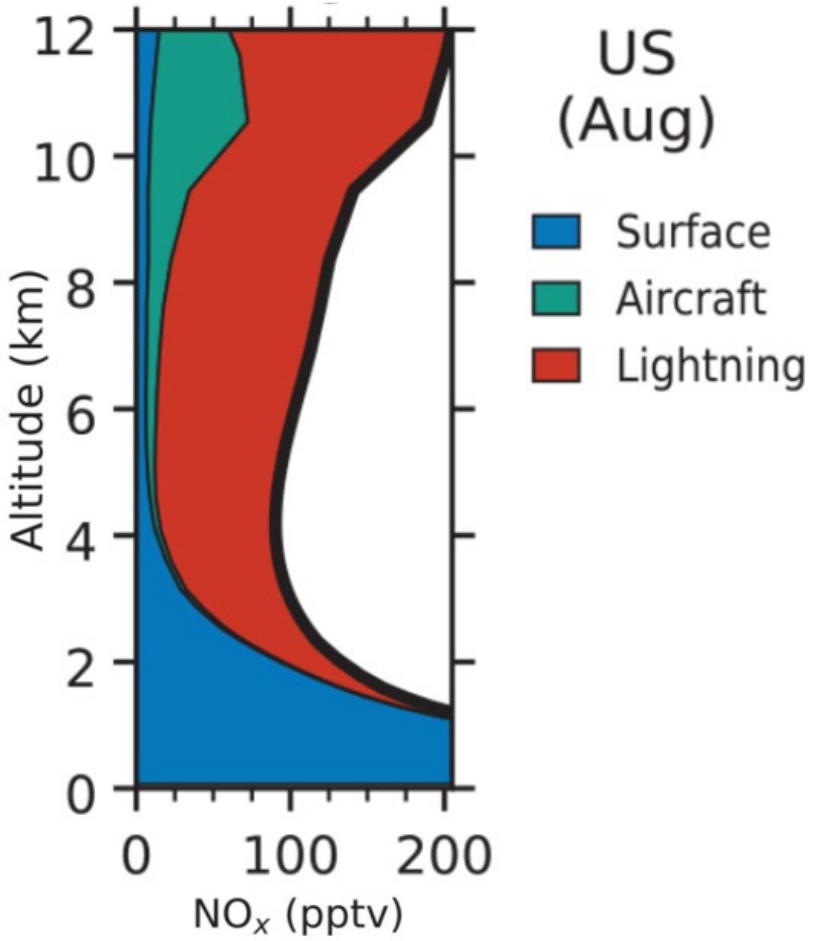
Baseline CAMx Configuration

- Ramboll processed **new** emissions for
  - Aircraft climb-out and cruise (EDGAR 0.1°× 0.1°)
  - Lightning NOx
  - MEGAN biogenics (using Daniel Huber's **updated Soil NOx parameterization**)

2022 Annual SNOx % Differences



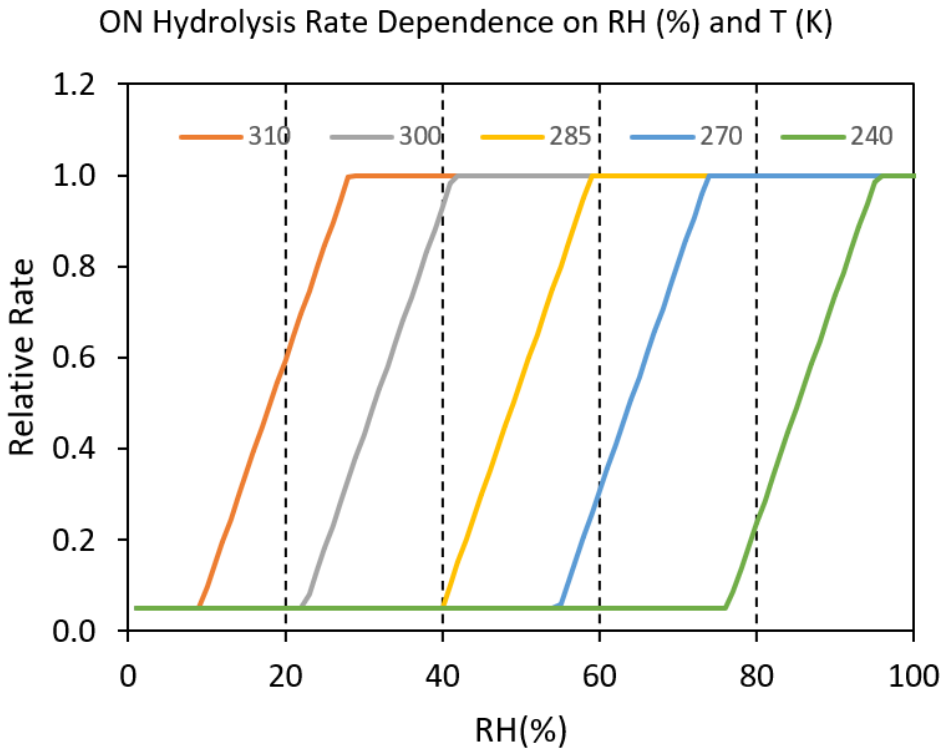
Ramboll 2025a; 2025b



Shah et al., 2023

CAMx Chemistry Update

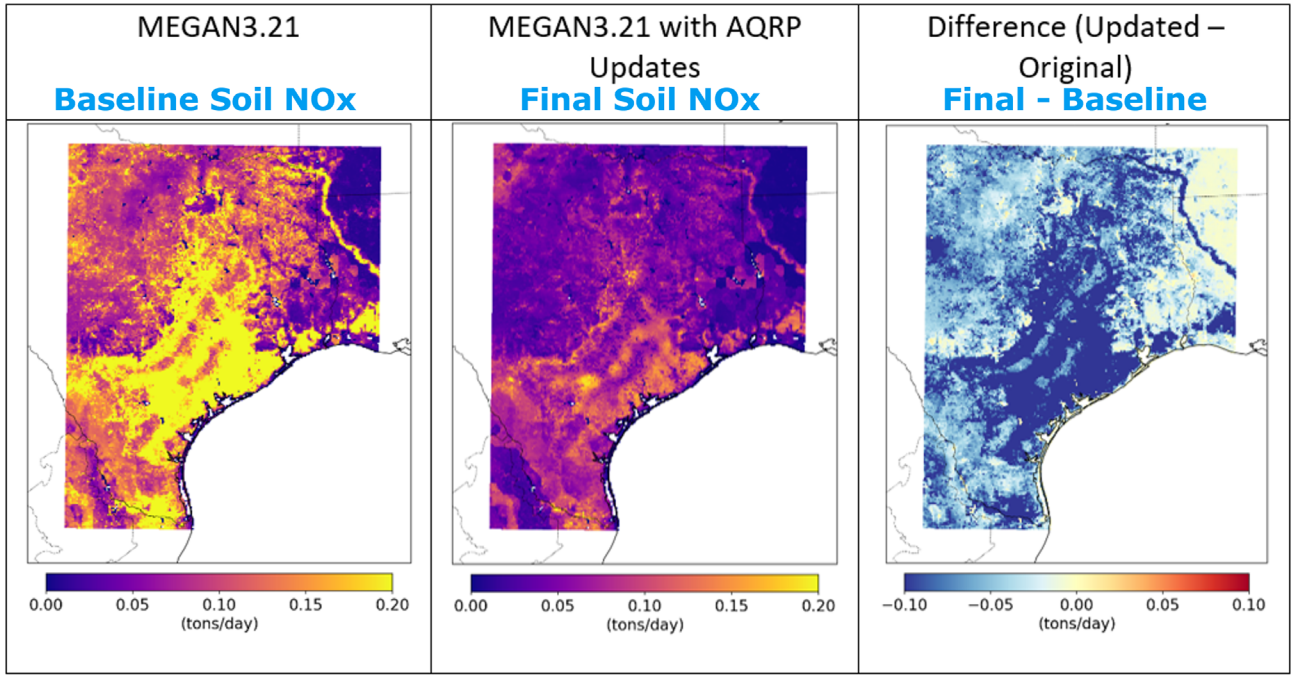
- Baseline CAMx uses unmodified CAMx v7.31
  - Simple parameterization of organic nitrate (ON) hydrolysis derived from Liu et al. (2012) and Rollins et al. (2013)
  - Hydrolyzed ONs unavailable for photolysis and/or OH reactions that regenerate NOx ("NOx recycling")
- Considered updates to NOx recycling from HNO3, *p*NO3 and ONs
  - Decided against enhanced *p*NO3 photolysis due to uncertainty in overall importance and ties to specific chemical interaction (e.g. aerosol Cl content)
- CAMx update focuses on ON hydrolysis update
  - Considers aerosol phase-state (and therefore temperature/humidity) without introducing any dependence on aerosol composition
  - Transition from glassy solid (Relative Rate=0.05) to liquid aerosol (1.0)
  - Used in Final CAMx run
    - Update showed near-zero impacts to surface NO_2 concentrations
    - Very minor impacts in the free troposphere and NO_2 column amounts



MEGAN Soil NOx Updates

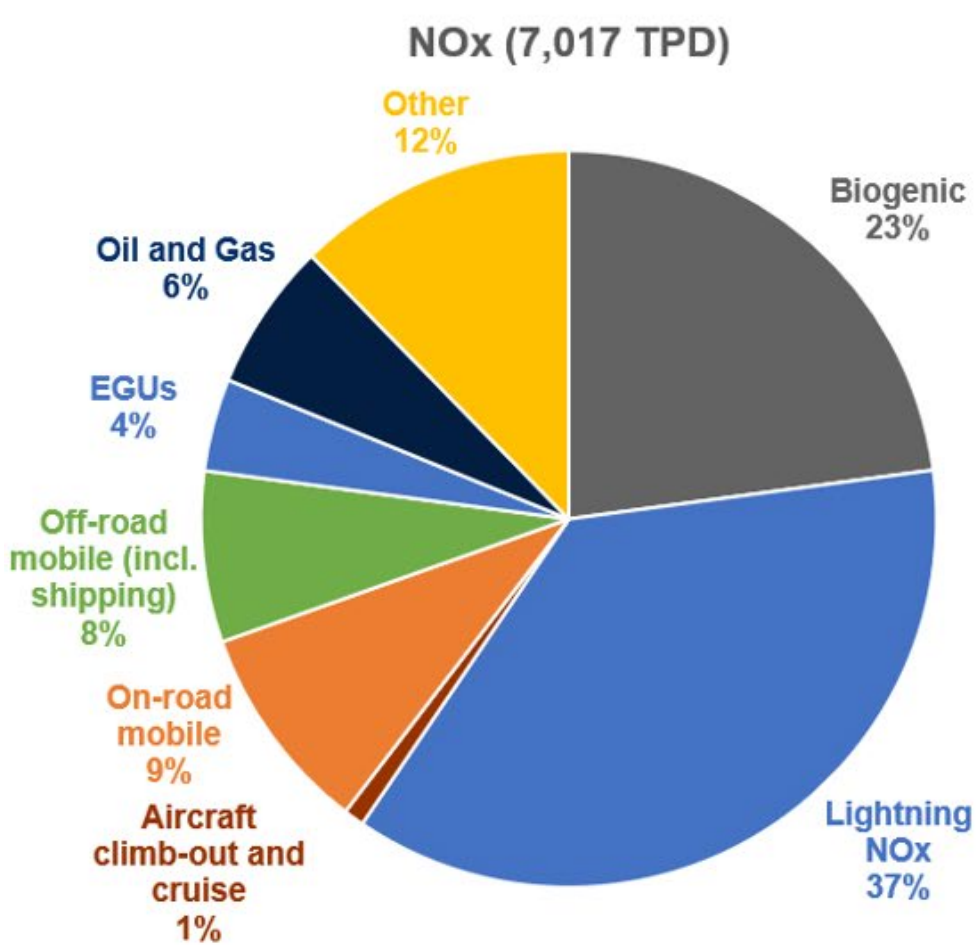
- Baseline CAMx uses MEGAN v3.21 with updated BDSNP for soil NOx emissions
  - Originally developed for Texas COG Rider 7 projects
  - Adds new temperature and soil moisture response functions
  - Updated nitrogen deposition and fertilizer application data
  - Addition of soil nitrous acid (HONO) emissions
- Baseline CAMx near-surface and satellite evaluation revealed soil NOx likely overestimated
- Final CAMx uses MEGAN v3.21 with updates to reduce soil NOx
  - Use WRF layer 2 soil moisture and temperature
  - Shortens decay period for soil N from fertilizer and N deposition half-life
  - Reduced soil HONO emissions to account for soil N availability (similar to existing reduction for soil NO)

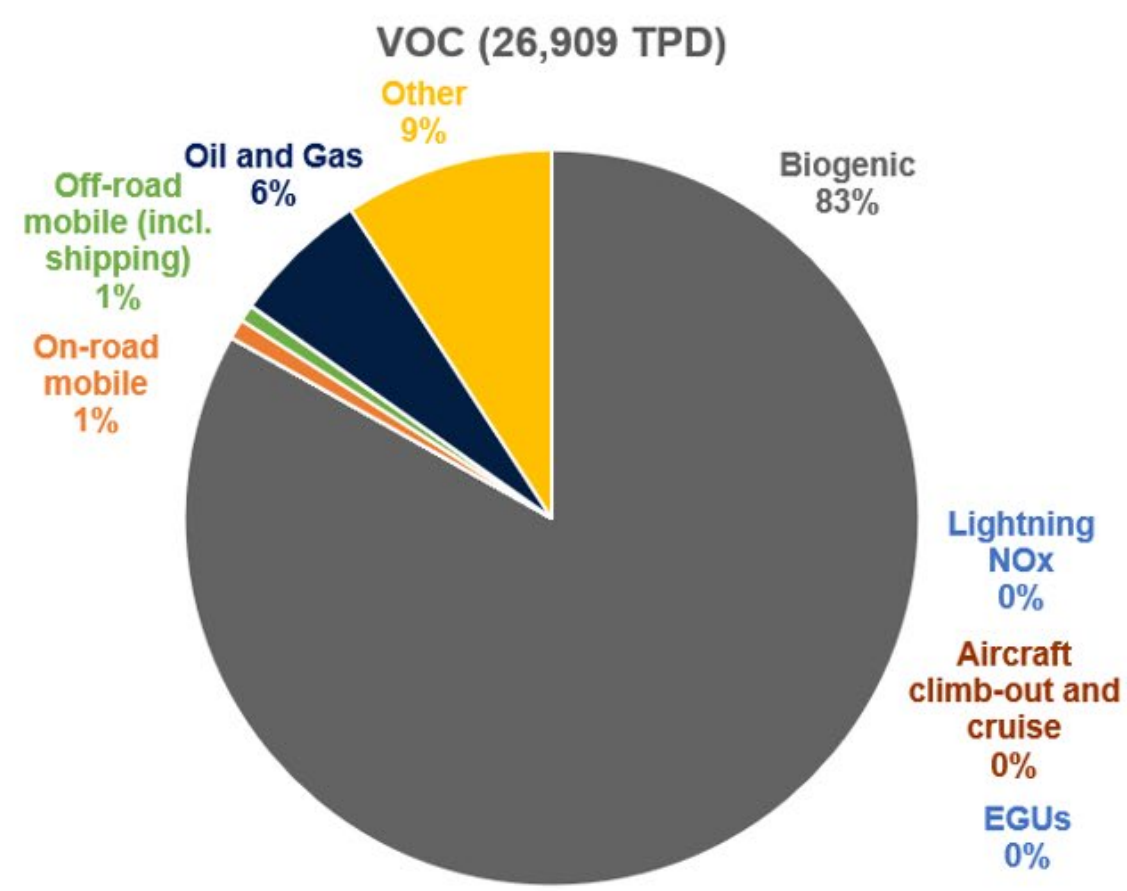
Species	Baseline Soil NOx (tpd)	Final Soil NOx (tpd)	Final – Baseline (% Change)
BVOC	21,797	21,848	0%
NOx (NO+HONO)	4,339	1,830	-58%



BDSNP: Berkeley Dalhousie Soil NOx Parameterization

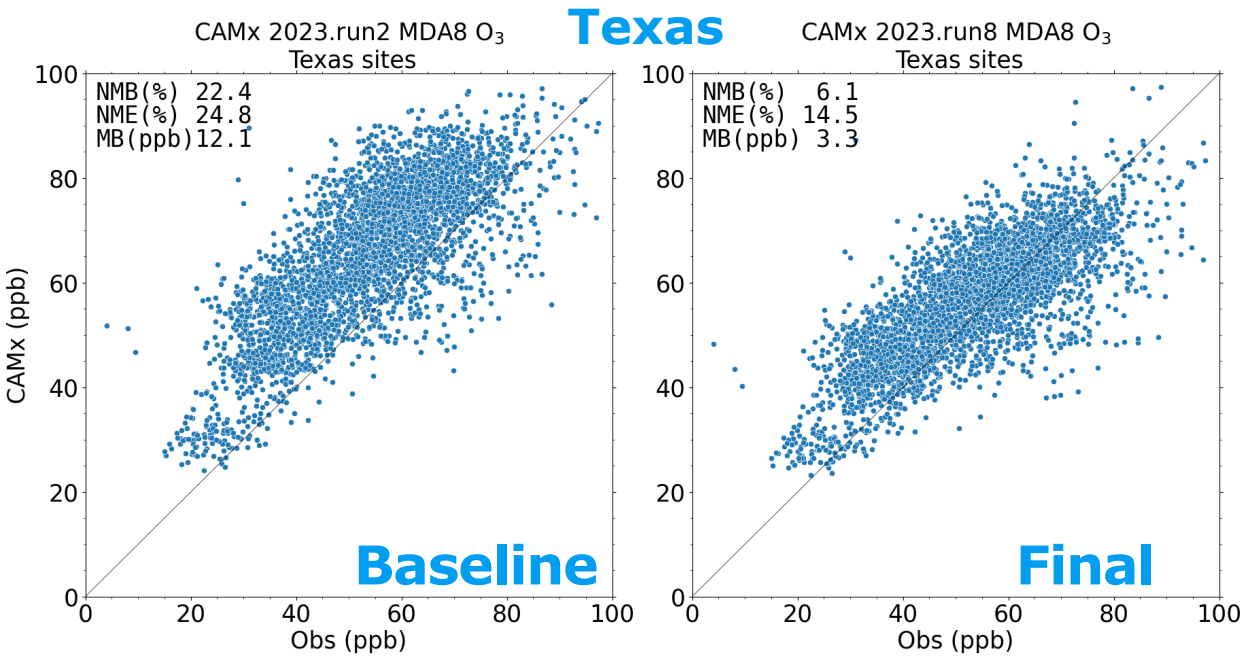
NOx and VOC Emission Summary for CAMx 4 km Domain (Final)

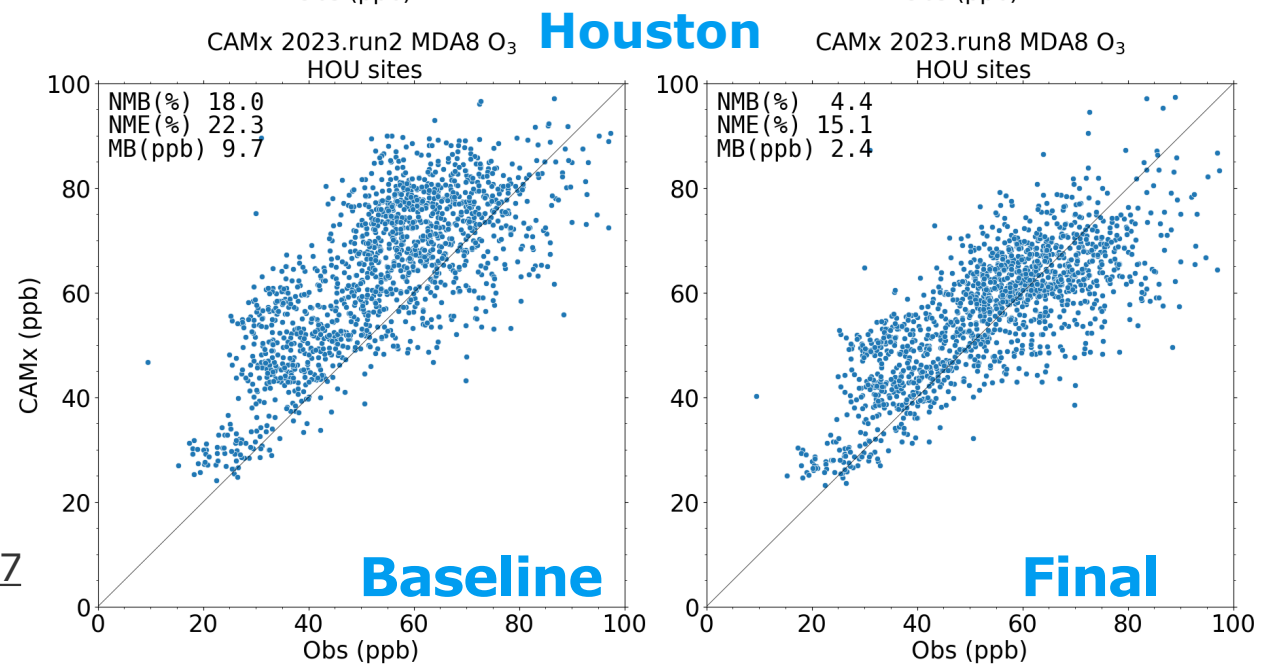




CAMx Ozone Model Performance

- Baseline CAMx ozone biased high across Texas
- Soil NOx adjustments in Final run show large improvements in bias and error
  - NMB (± 5%) and NME (< 15%) within or near Goal benchmark*
- Similar results in Dallas and San Antonio

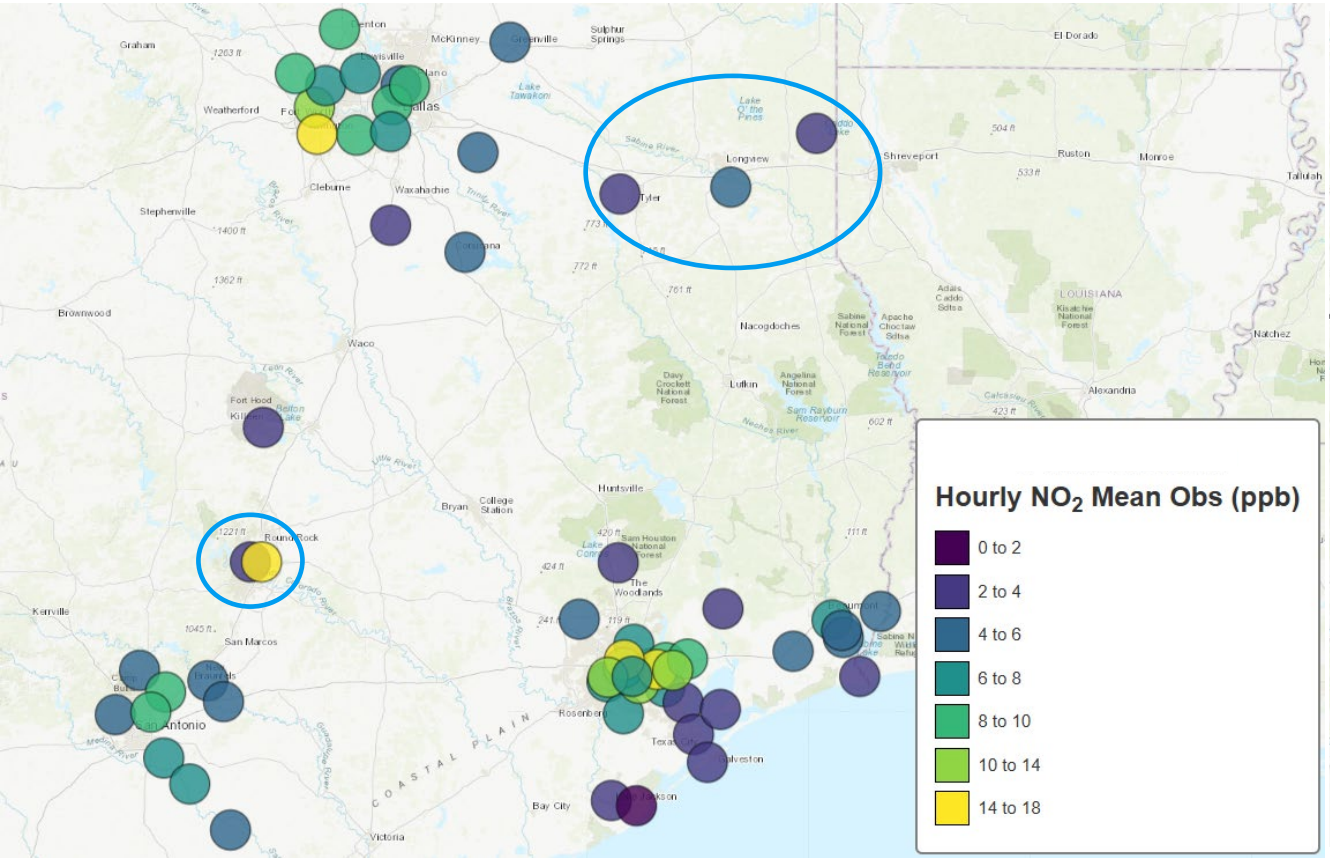




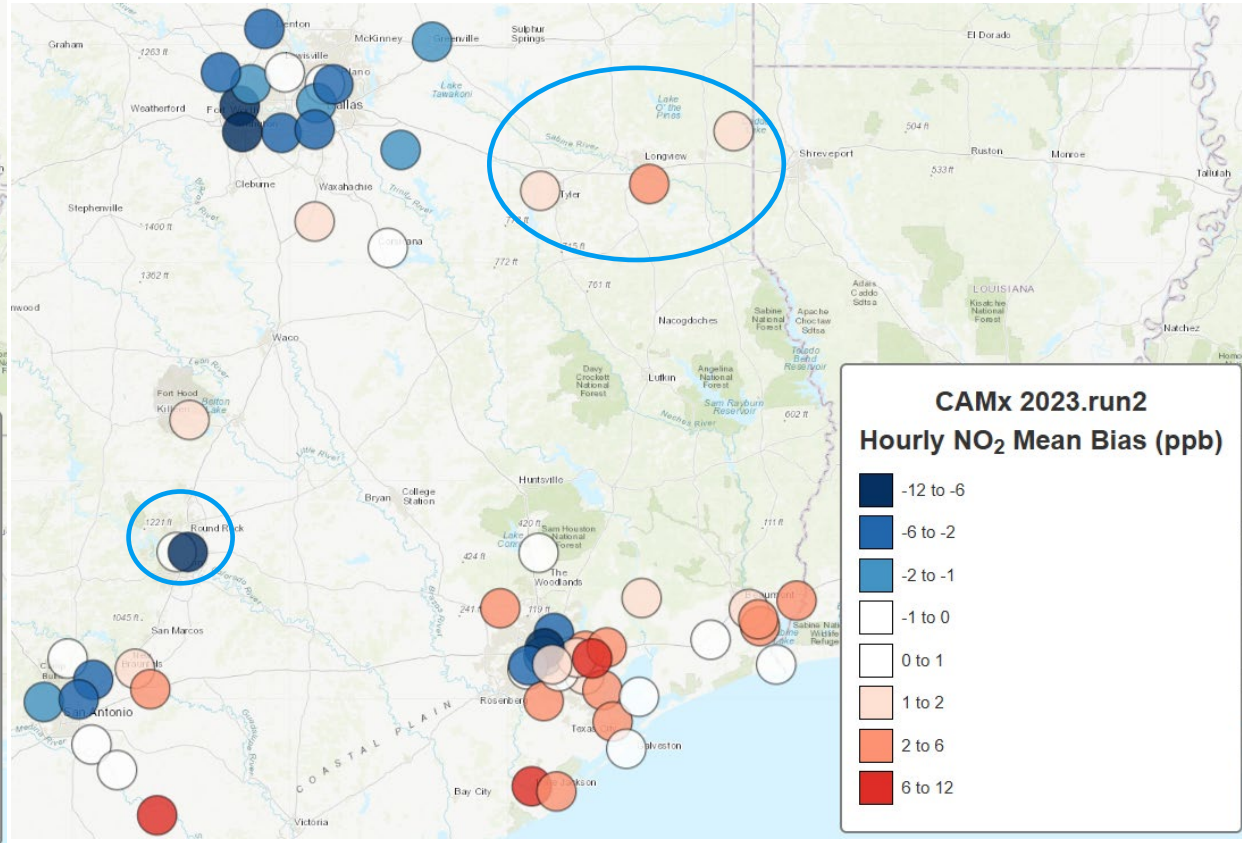
*Emery et al., 2017

CAMx NO_2 Model Performance (8 AM – 6 PM CDT)

NO_2 Mean Observation (ppb)



CAMx Baseline Mean Bias (ppb)



- Urban and near-roadway monitors have largest negative biases
- Rural monitors show positive biases

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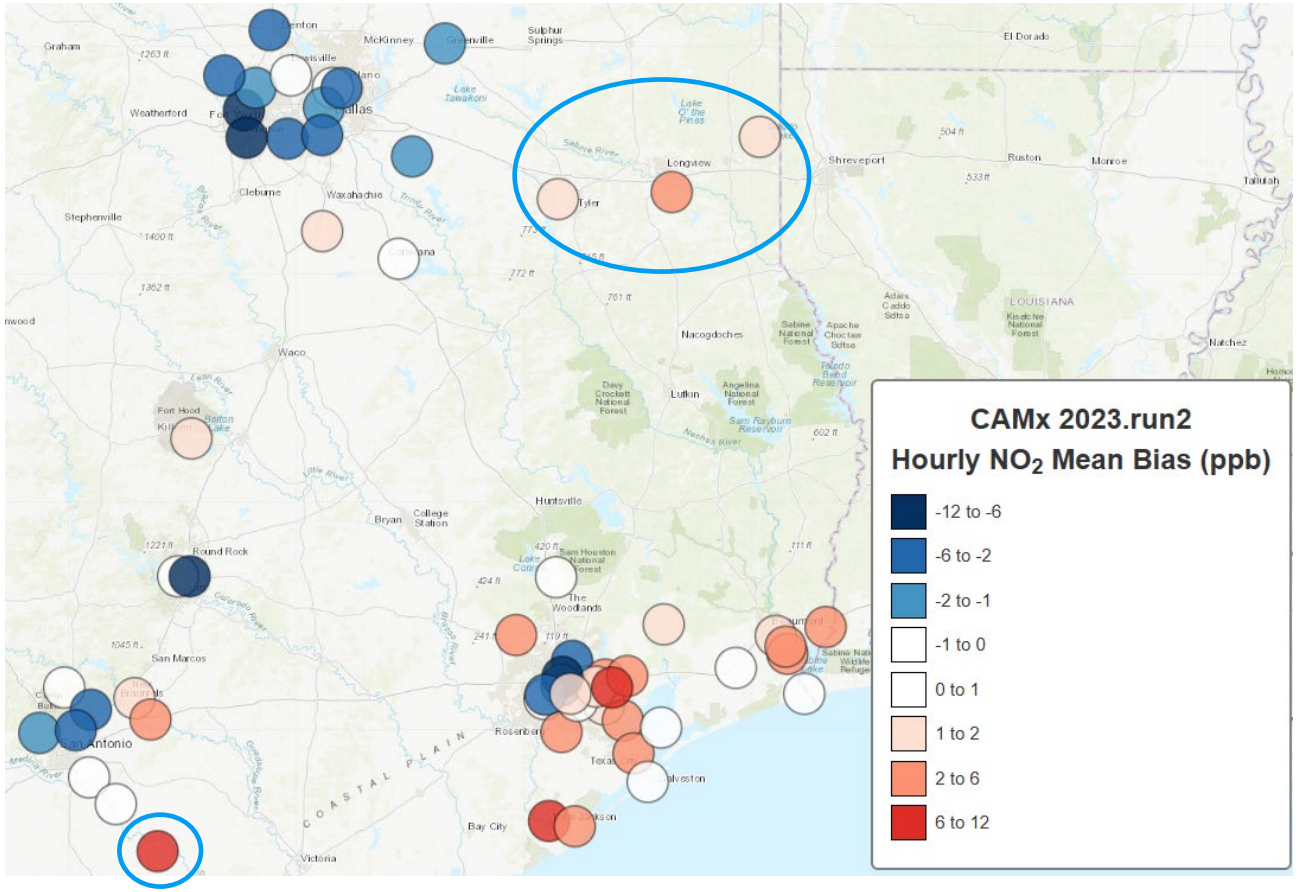
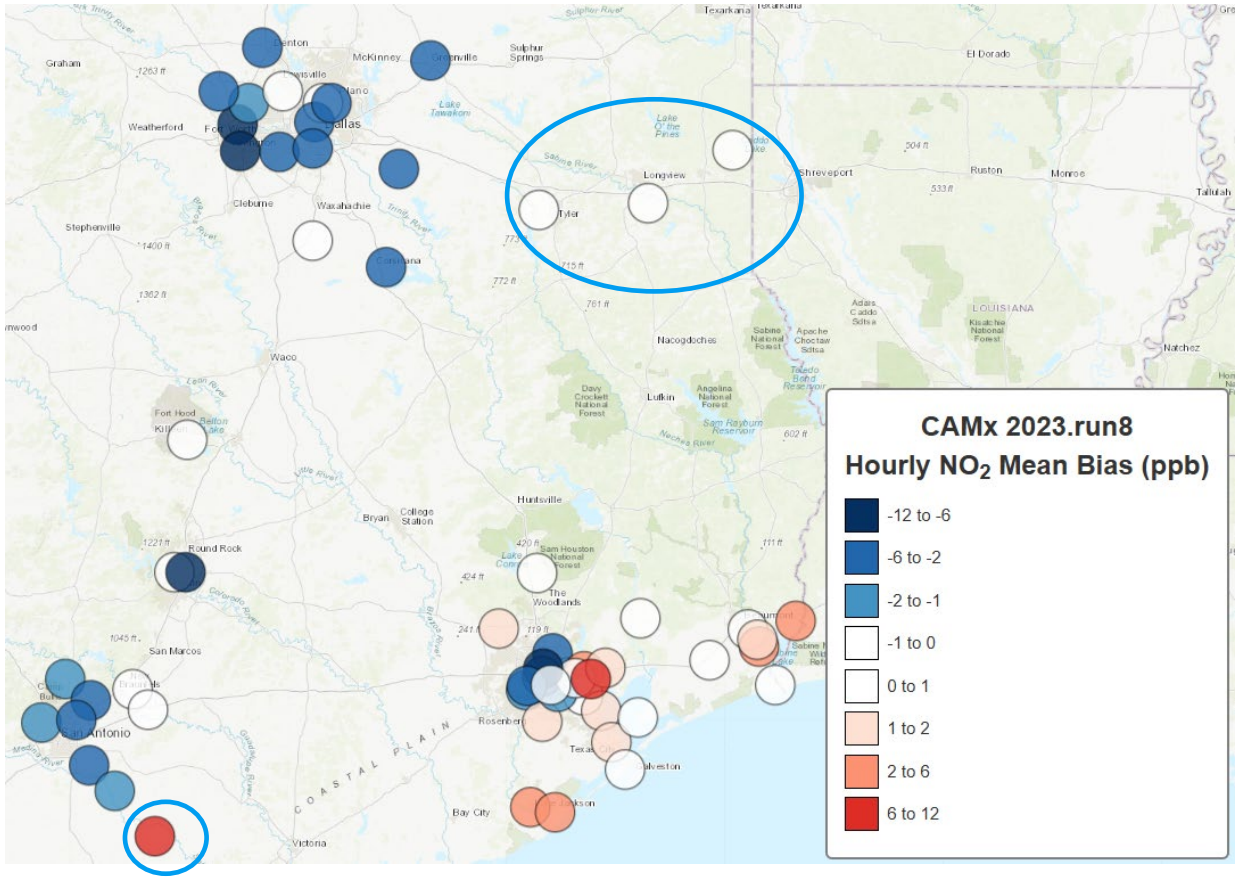
CAMx NO_2 Model Performance (8 AM – 6 PM CDT)

CAMx Baseline Mean Bias (ppb)



CAMx Final Mean Bias (ppb)



- Positive bias reduced in some rural locations (Northeast Texas, e.g.)
- Large positive biases remain in some O+G regions (Karnes County C1070 in Eagle Ford Shale)

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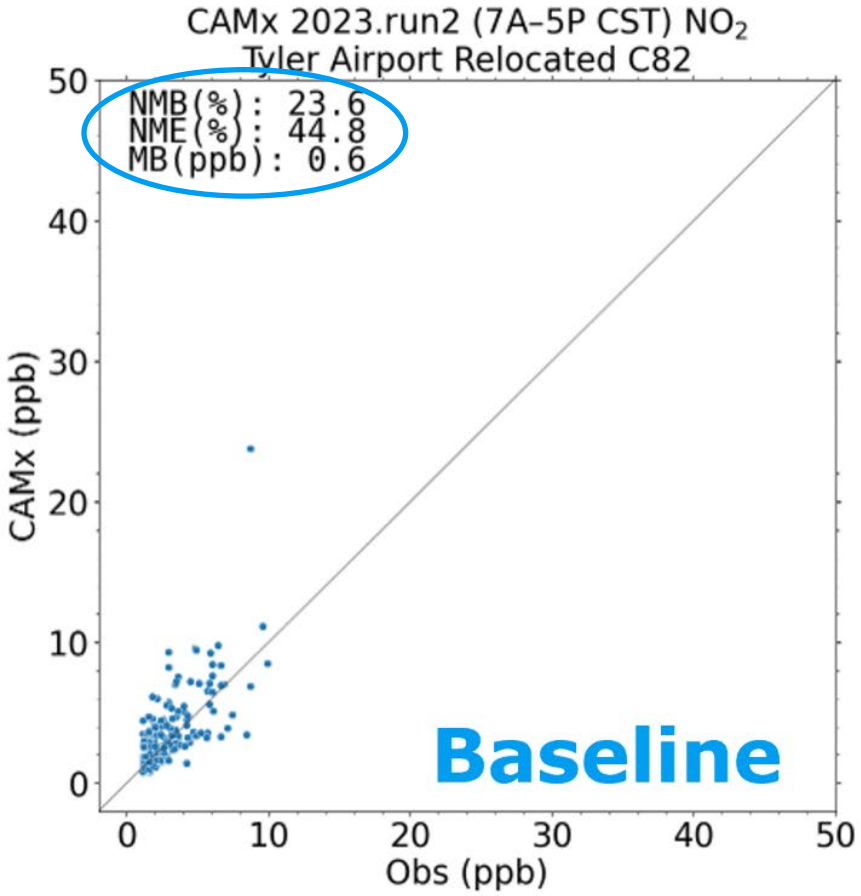
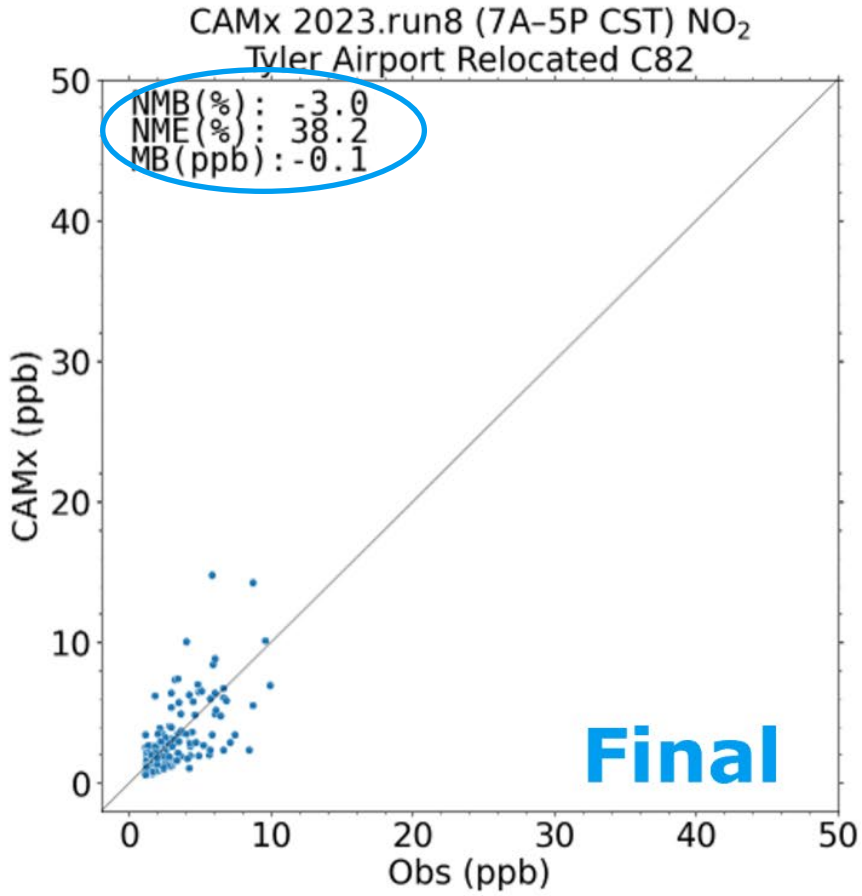
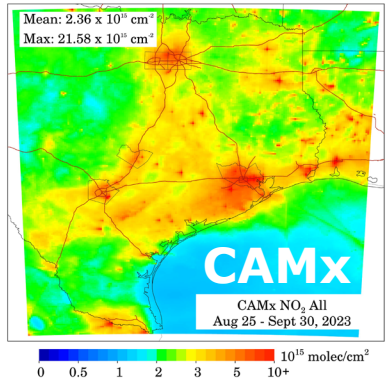
CAMx NO_2 Model Performance at Tyler (8 AM – 6 PM CDT)

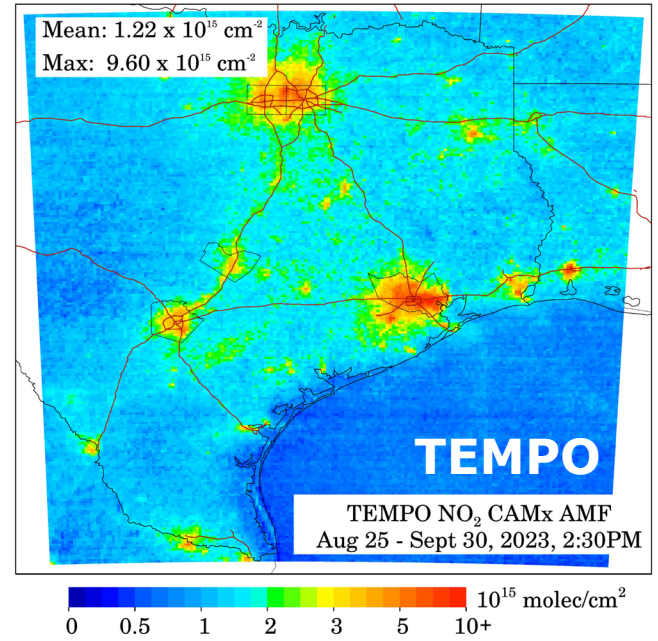
- During 2023, high-NOx instrument collected NO_2 measurements adjacent to TCEQ's NOx instrument at Tyler Airport (CAMS 82) in Northeast Texas
- MEGAN soil NOx updates in Final CAMx run improve agreement with NO_2 observations

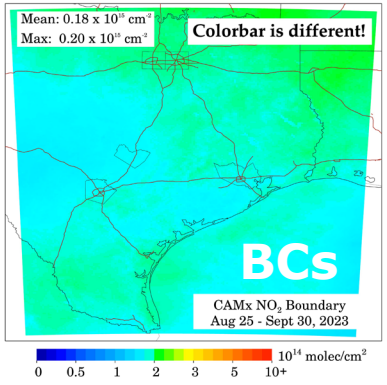


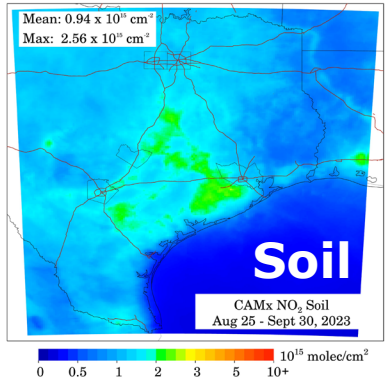


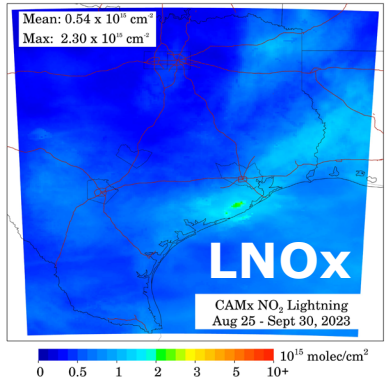
Tagged CAMx NO_2 Columns compared with TEMPO NO_2 Columns

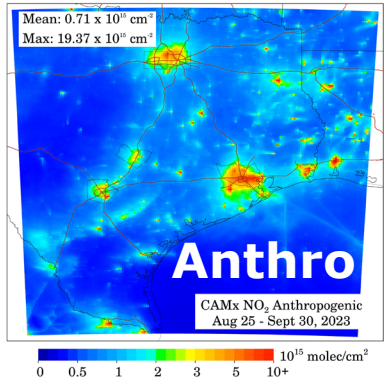


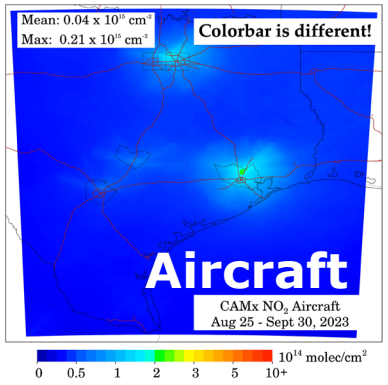


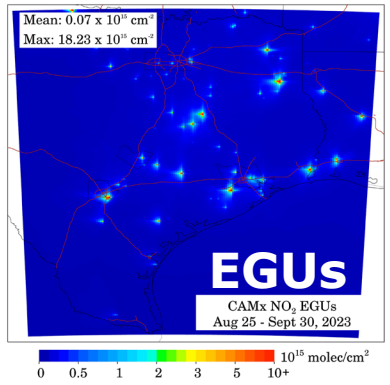


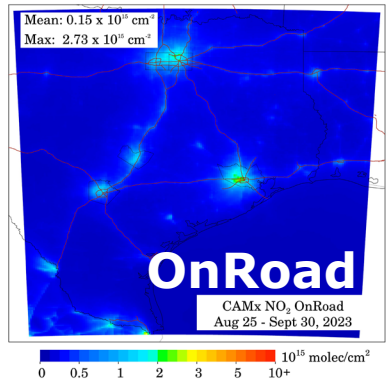


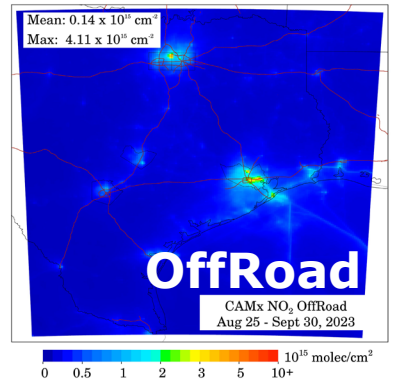


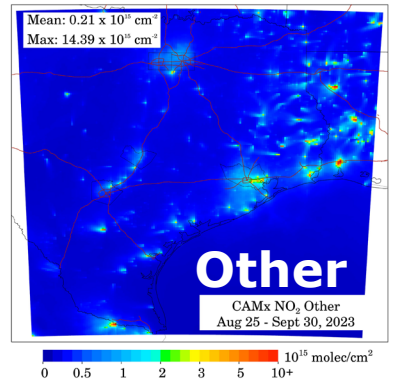


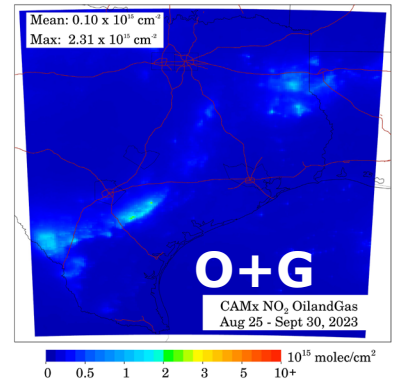






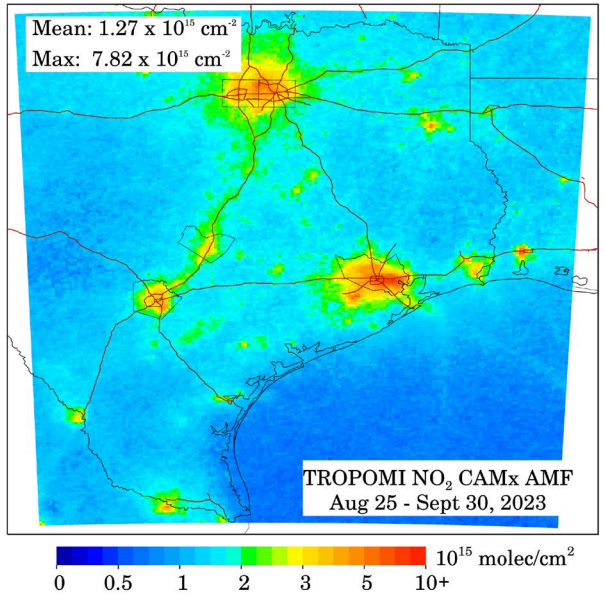




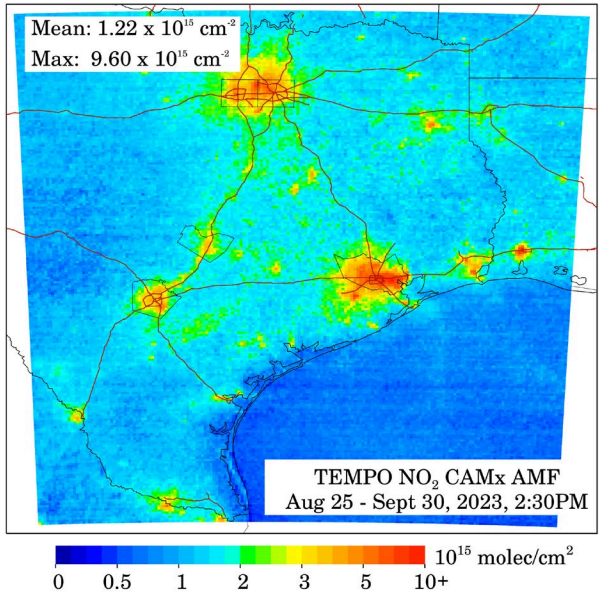


TEMPO and TROPOMI NO_2 Columns

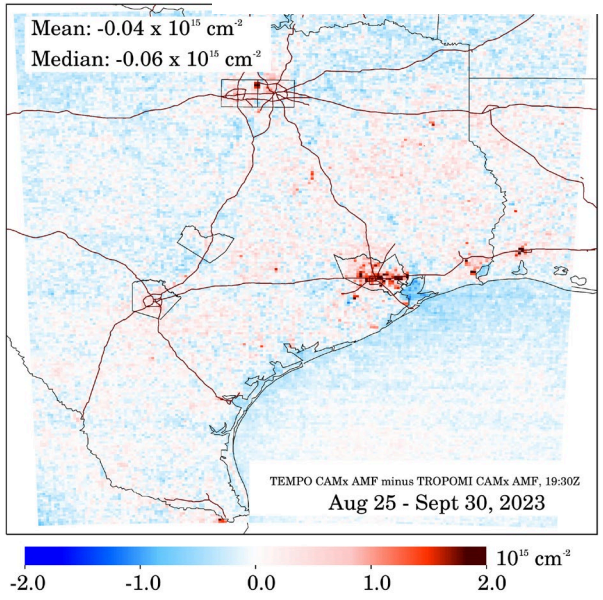
TROPOMI NO_2



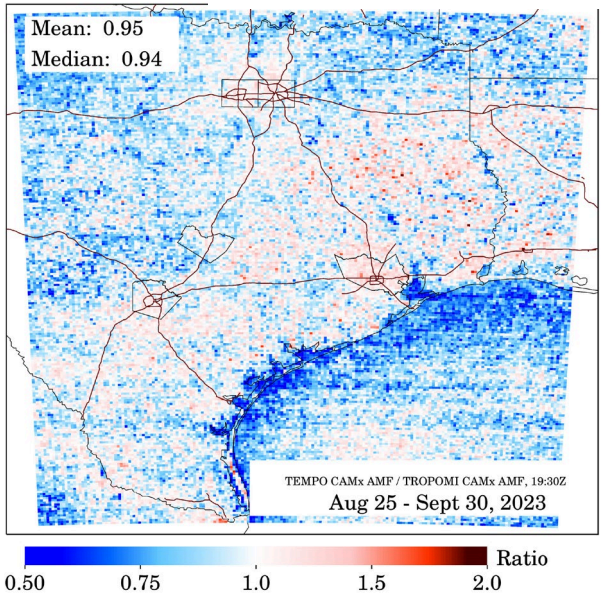
TEMPO NO_2 2:30 PM



TEMPO-TROPOMI



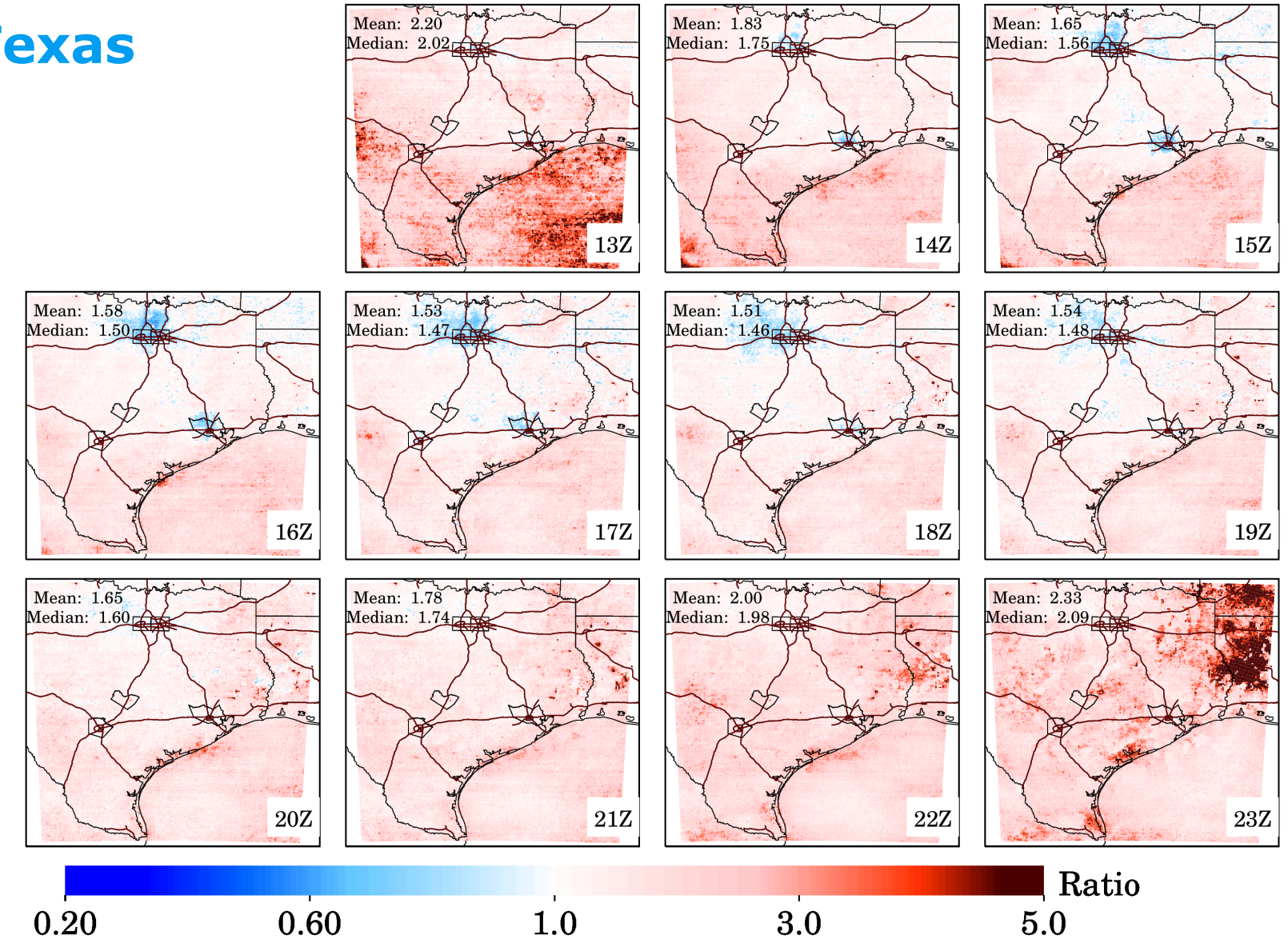
TEMPO/TROPOMI



- TEMPO NO_2 +10 to +20% larger in urban areas, especially Houston (likely due to TEMPO's higher spatial resolution)
- TEMPO NO_2 marginally lower (~5%) in rural areas
- TEMPO NO_2 has largest differences by ratio along the Gulf coastline
  - Feature present along all coastlines; artifact of surface reflectivity issue?
  - Likely updated in future TEMPO releases

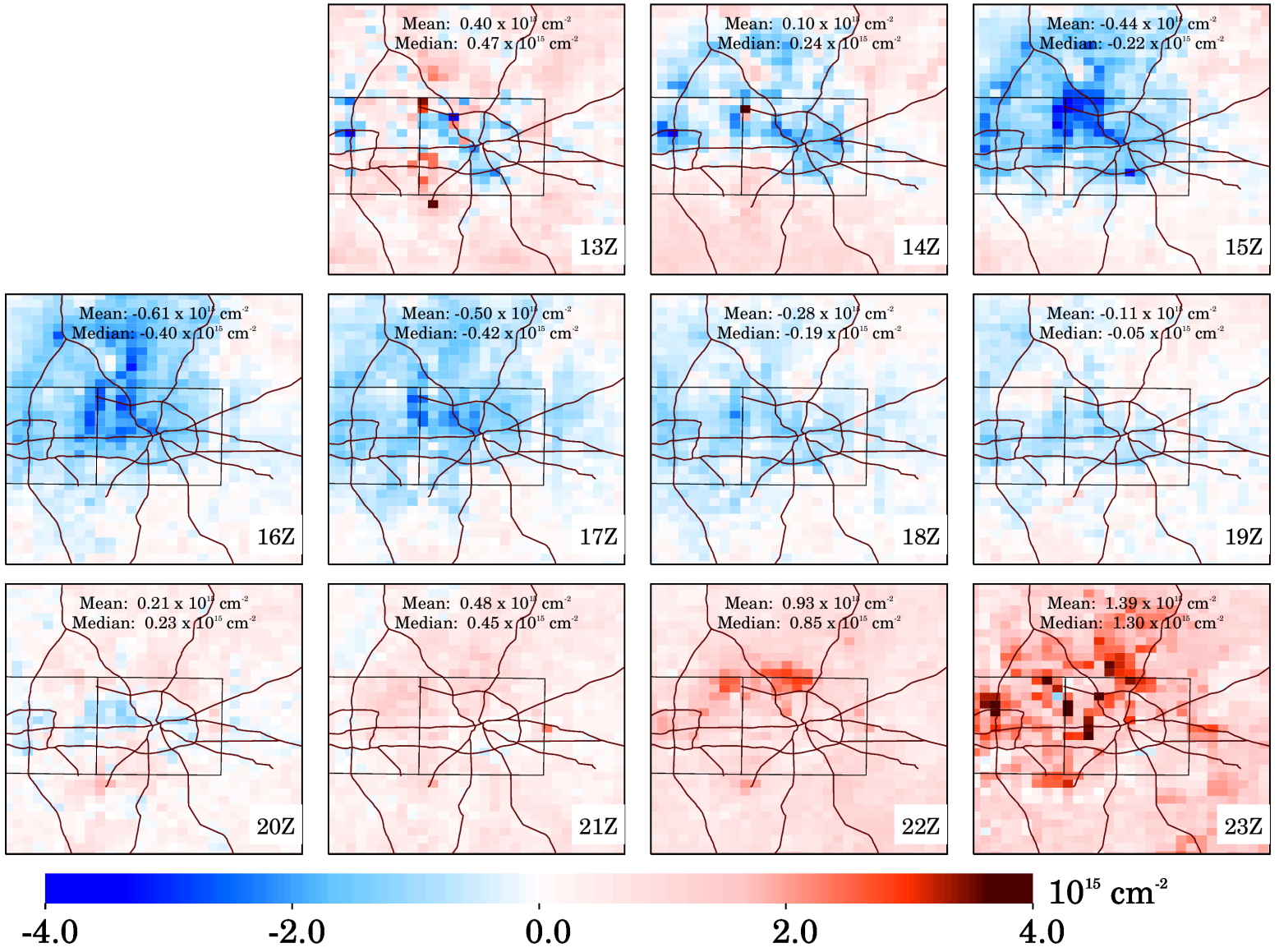
CAMx/TEMPO over East Texas
8 AM – 6 PM CDT

- CAMx NO_2 broadly larger than TEMPO NO_2 likely due to natural (LNOx and biogenic) sources
- However, CAMx NO_2 in urban areas during morning show an underestimate
- More uncertainty with low sun angle



CAMx/TEMPO over Dallas
8 AM – 6 PM CDT

- AM: substantial underestimate
  Late PM: overestimate
- Best agreement at the TROPOMI overpass time (19Z and 20Z)!



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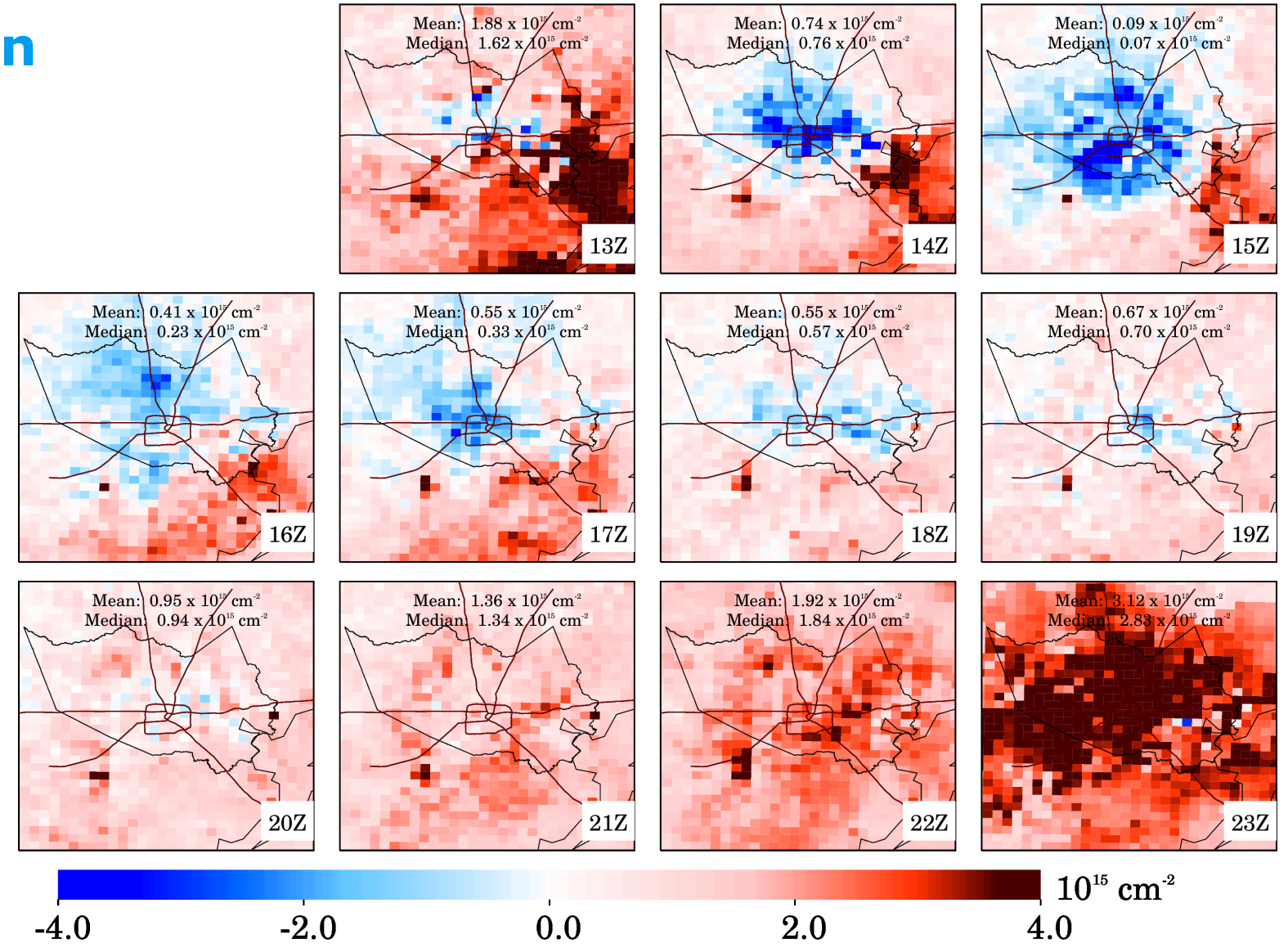
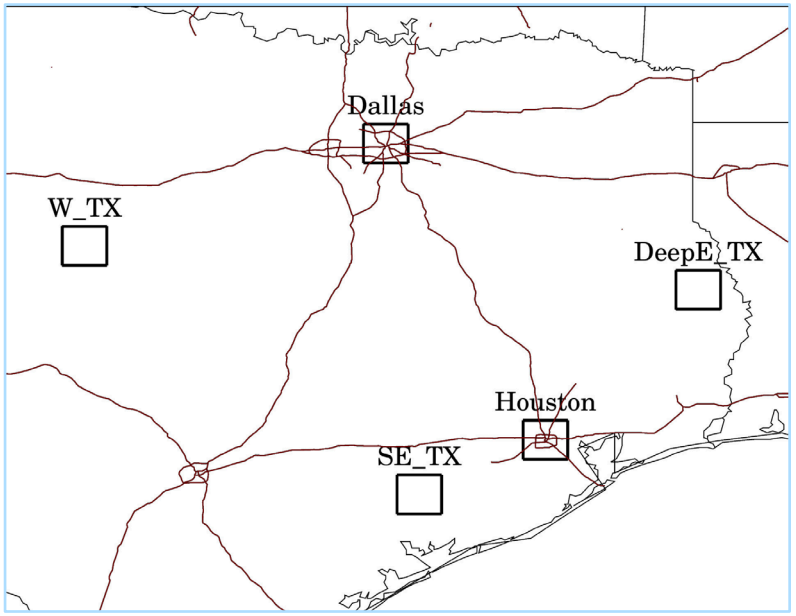
CAMx/TEMPO over Houston
8 AM – 6 PM CDT

- AM: substantial underestimate
  Late PM: large overestimate
- Best agreement in early afternoon
- EGU emissions use 2019 CEM data



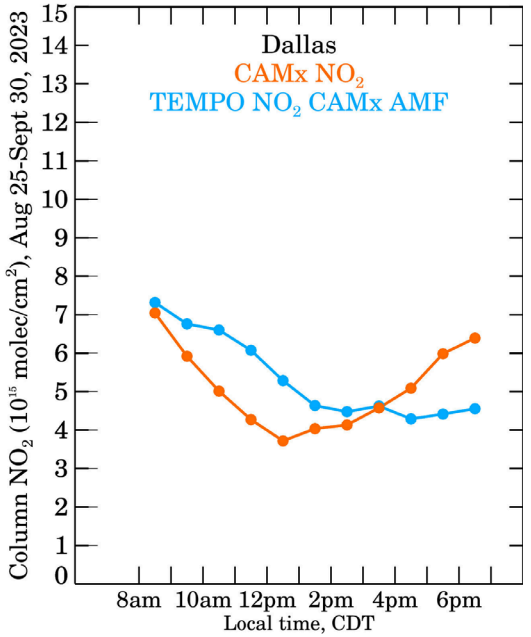
TEMPO and CAMx NO_2 Columns

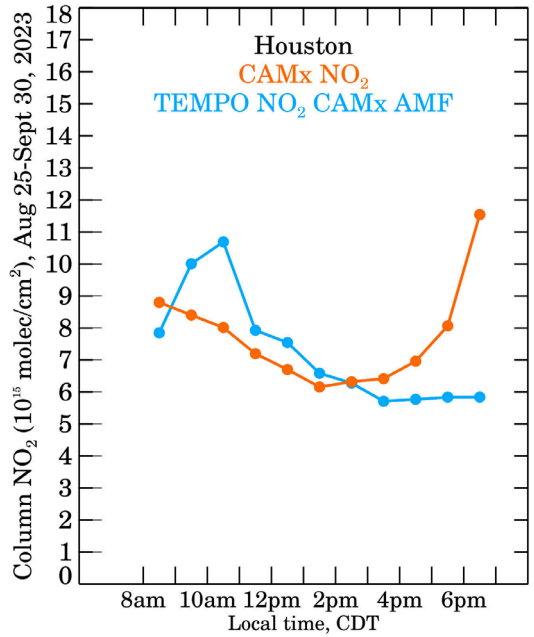


Urban areas

Mid-AM: Low CAMx NO_2

Late PM: High CAMx NO_2



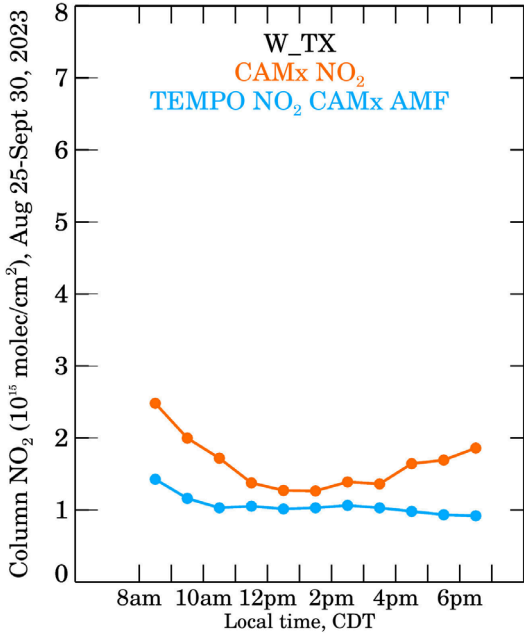


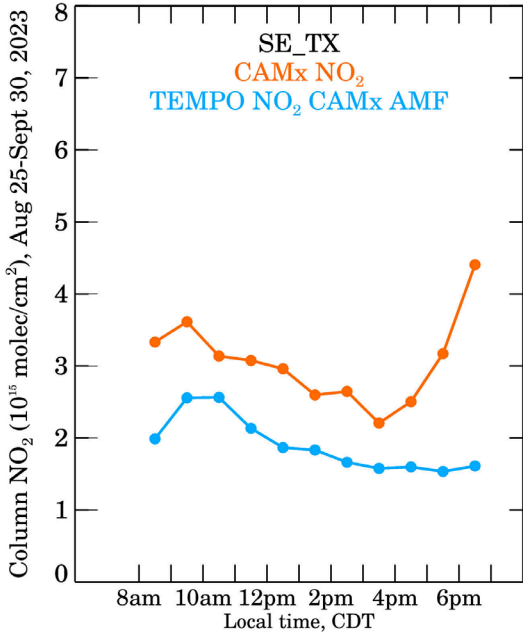
Rural areas

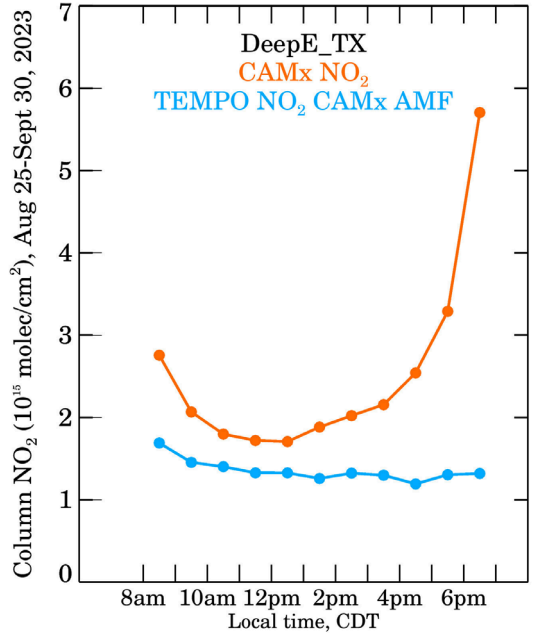
All hours: High CAMx NO_2, largest differences in early AM and late PM

Dallas, Houston, SE_TX, DeepE_TX

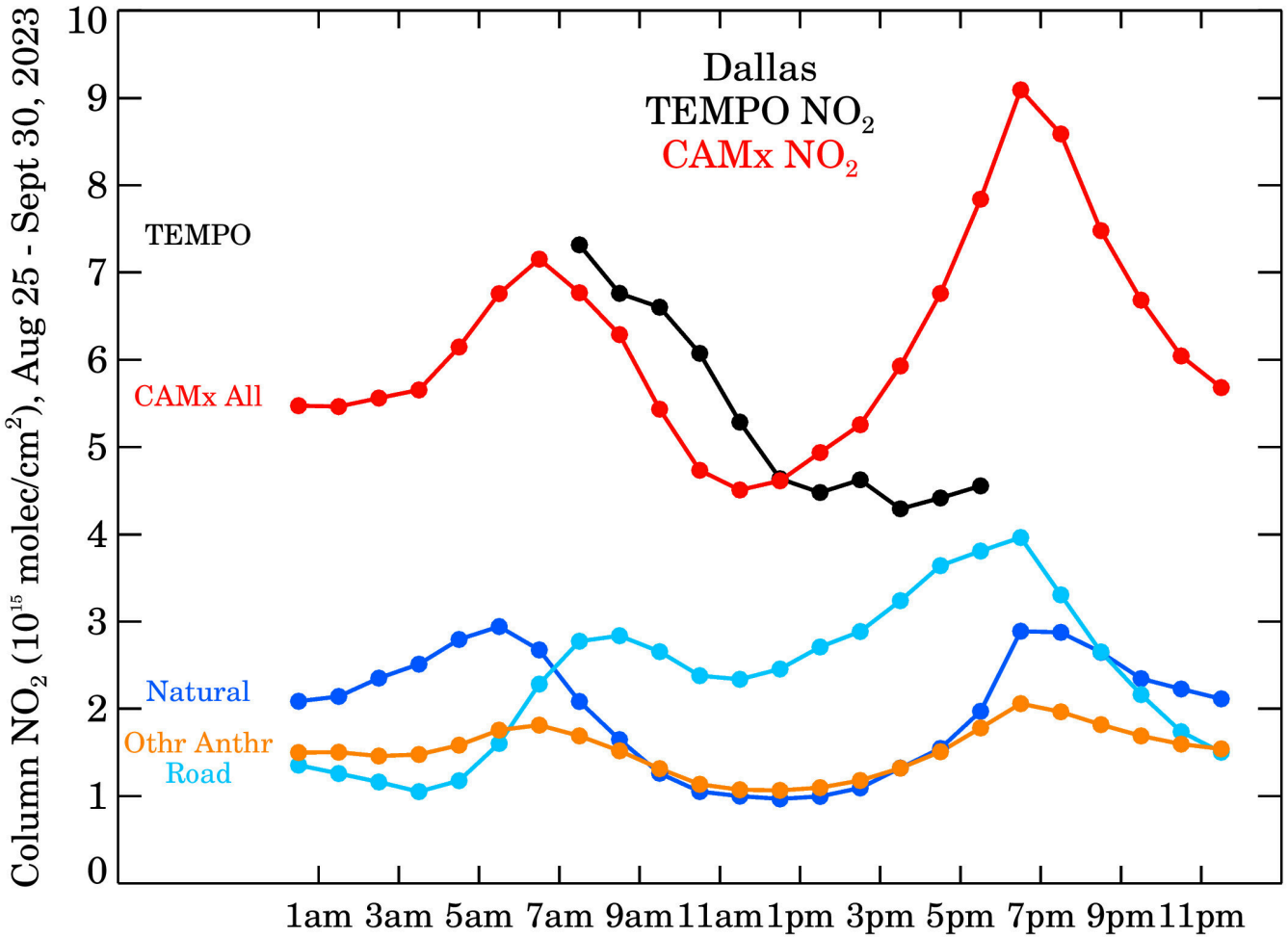
CAMx late PM spike mostly from lightning NOx







TEMPO and Tagged CAMx NO_2 Columns: Dallas



- Late PM disagreement could be due to
  - PBL dynamics
  - Lightning NOx
- Increase in On-road NO_2 throughout day with peak around 6 PM (NOx emissions peak about 2 hours earlier)
- Are diesel vehicle emissions underestimated?
- Natural (Lightning and Soil) NOx also generally larger than expected

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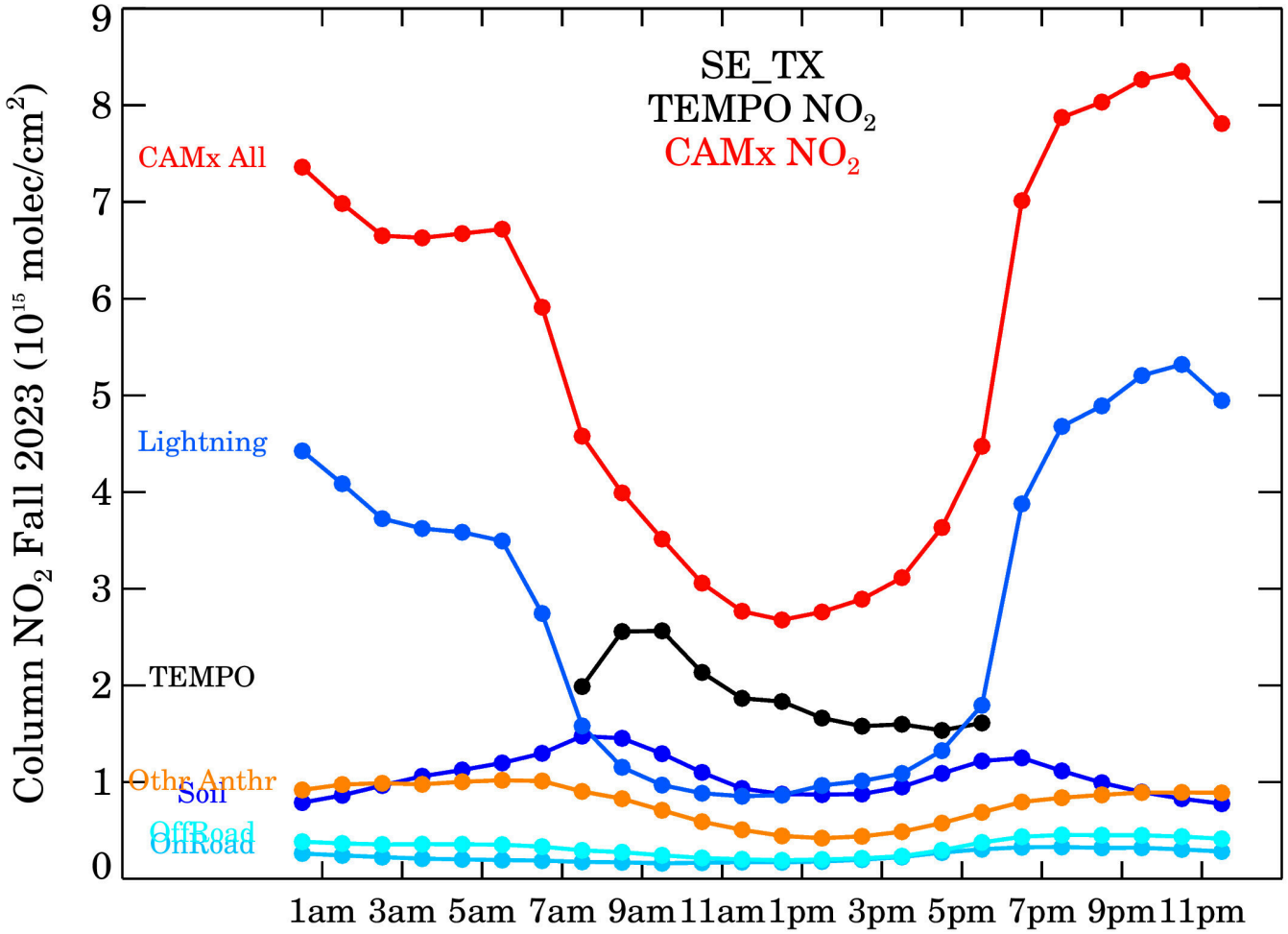
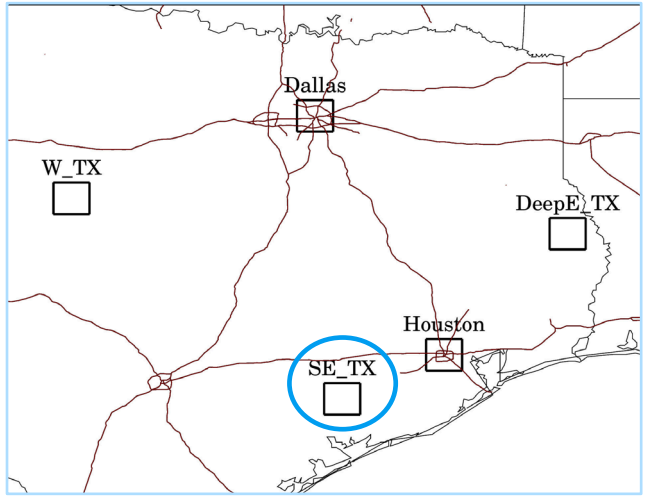
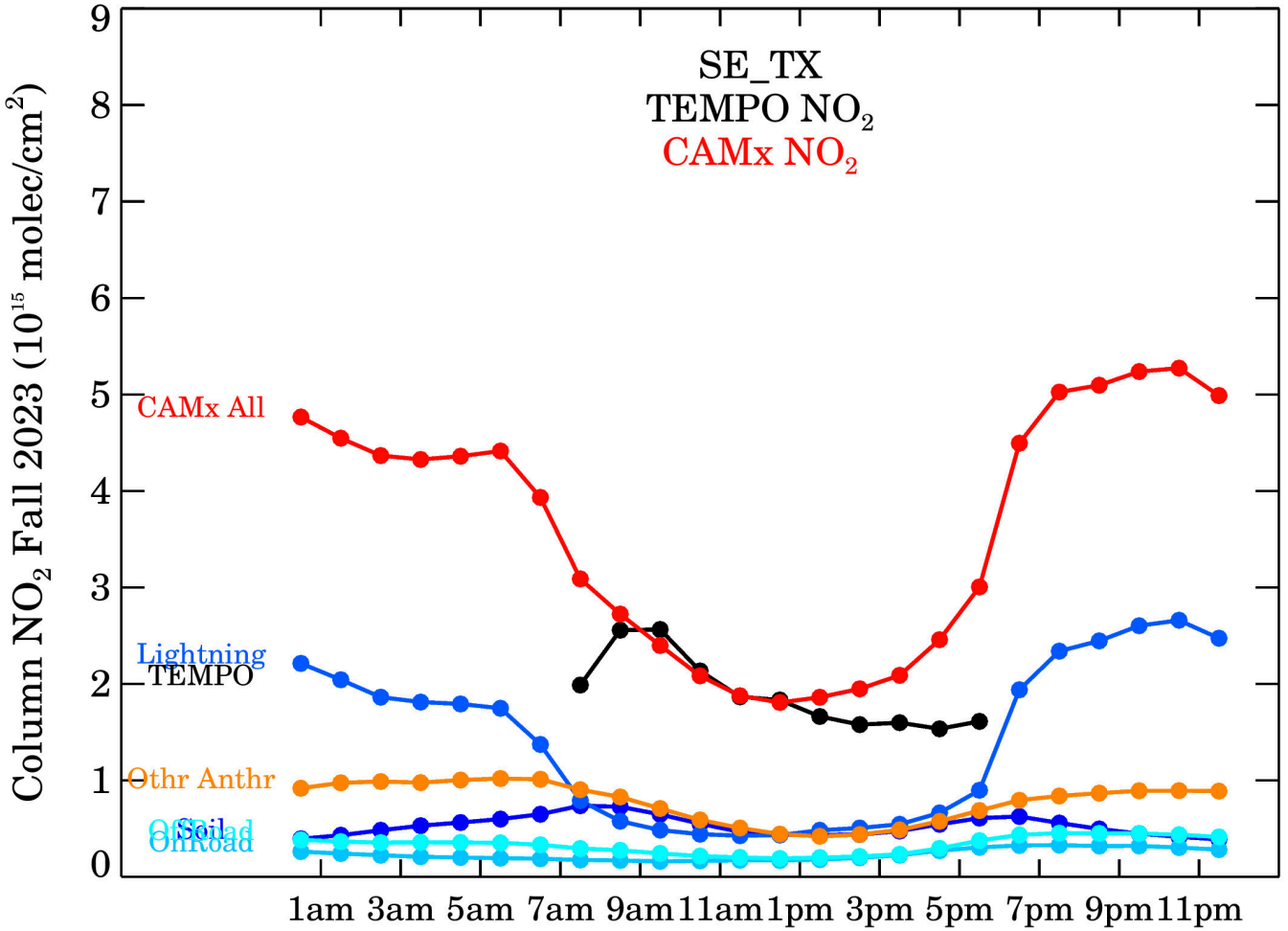
TEMPO and Tagged CAMx NO_2 Columns: Southeast TX



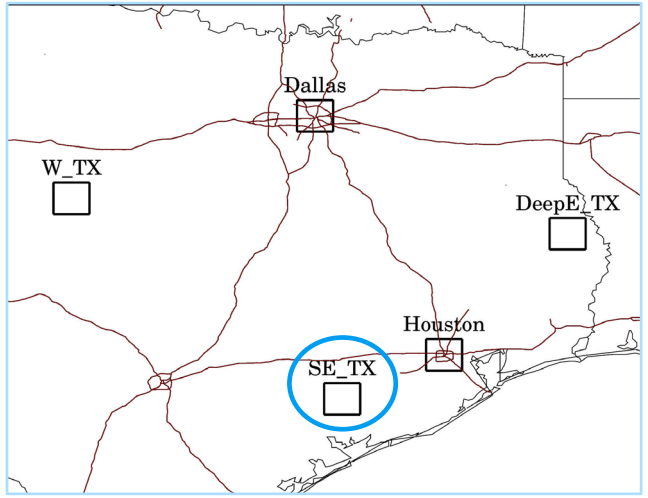
- Natural NOx (Lightning and Soil) generally larger than expected
- Evidence for a further reduction of soil and lightning NOx emissions



TEMPO and Tagged CAMx NO_2 Columns: Southeast TX



- Artificially halving both lightning NO_2 and soil NO_2 shows better agreement
- Late PM CAMx overestimate is still present, but improved



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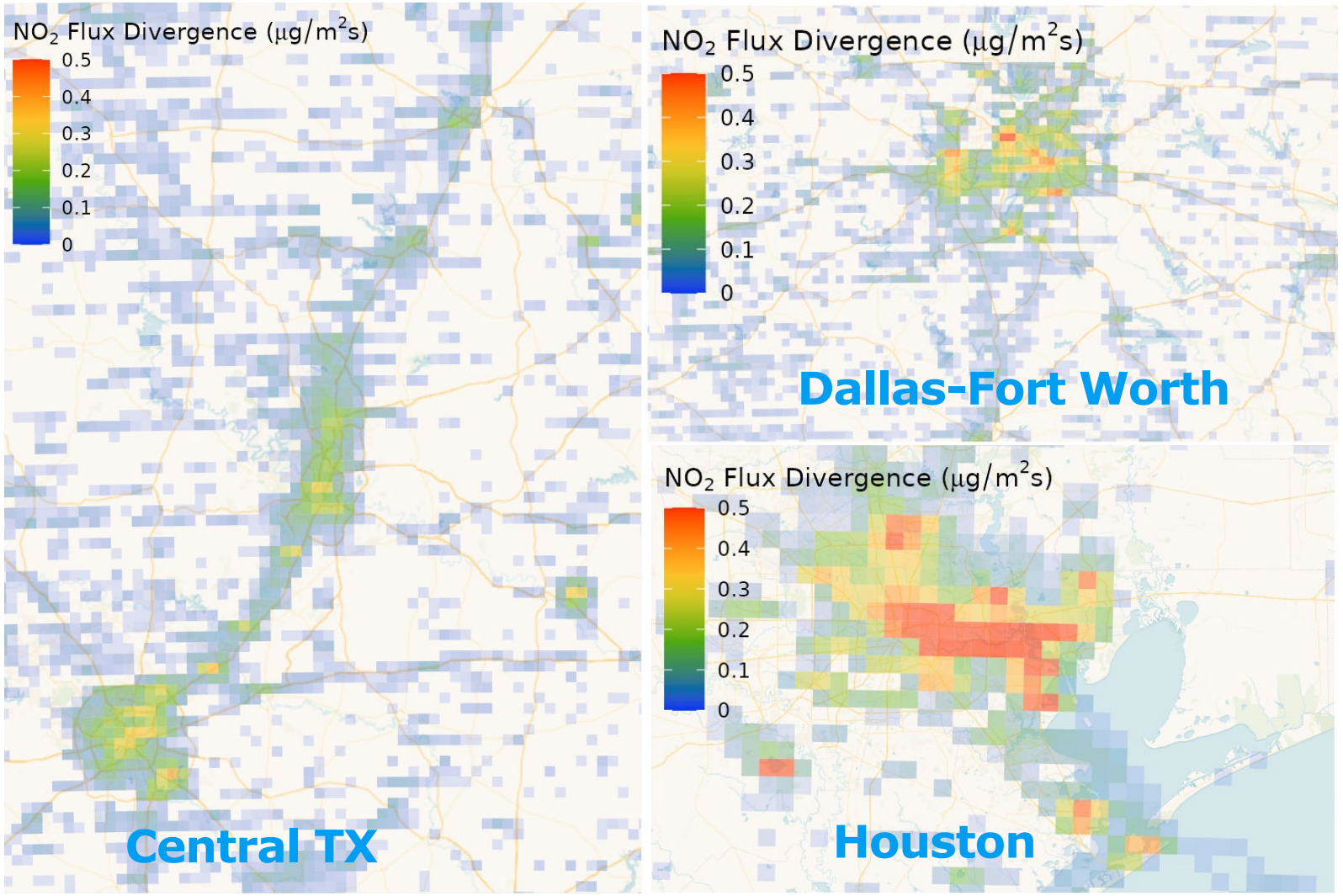
Flux Divergence using TEMPO NO_2 Columns

- First application of this method to TEMPO data, to our knowledge
- Slant column densities (SCDs) used to remove "boxy" artifacts of coarse GEOS-CF *a priori*
- Clearly identifies cities and large point sources
- Many highways show up as line sources – an improvement on TROPOMI-based FD results
- Caveat: resolving these features requires long sampling period
  - August 2023 – March 2025



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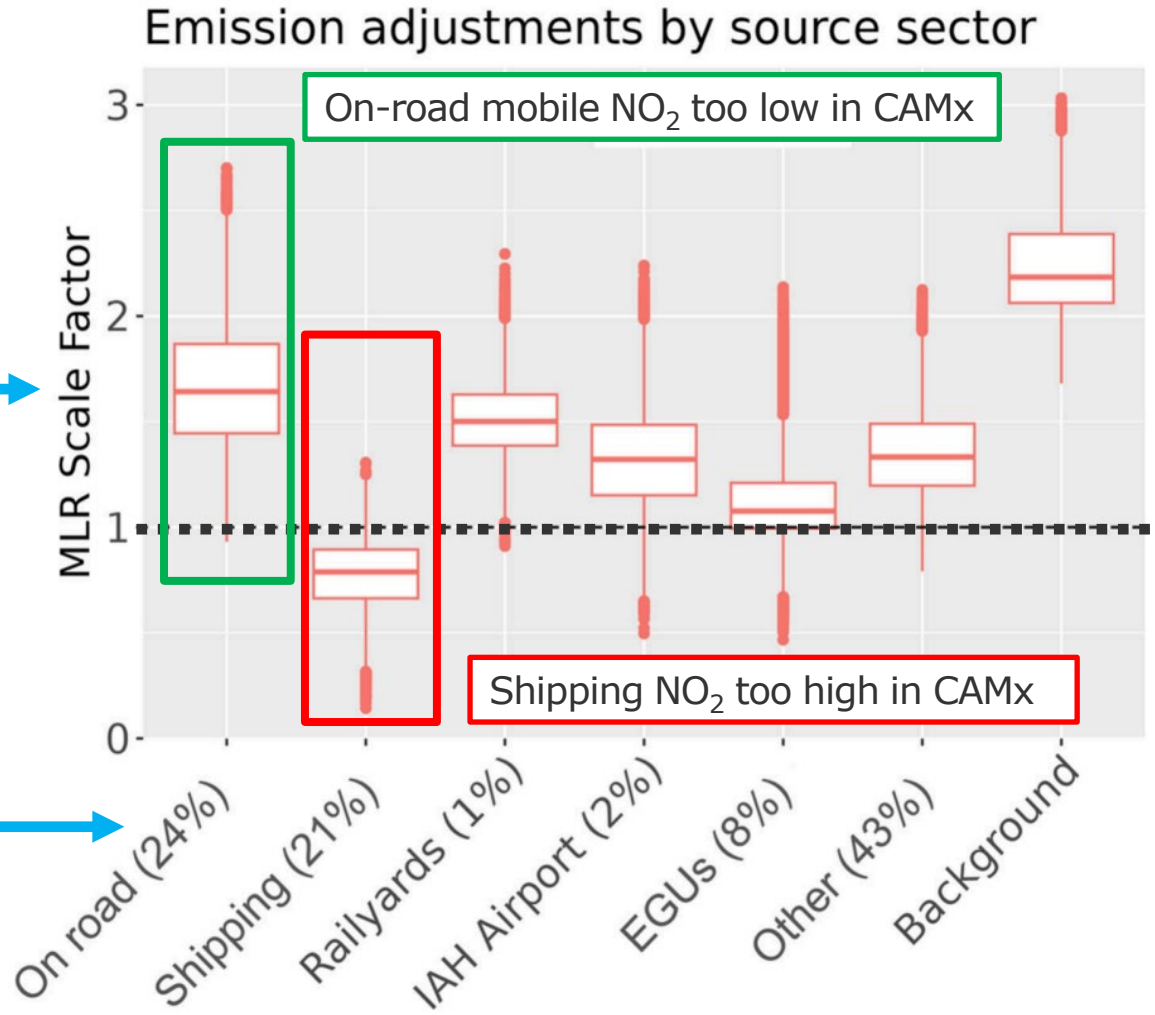
Multiple Linear Regression (MLR) Background – From AQRP 22-023

- Satellite and aircraft measurements can
  - Overcome the limited spatial coverage of surface monitoring sites
  - Help improve EIs and/or models
- Figure from AQRP 22-023 Houston TRACER-AQ Project using GCAS aircraft and tagged CAMx NO_2
- Figure showing **scale factor** needed for CAMx tagged NO_2 to replicate aircraft measured NO_2 in Houston
- Powerful statistical methods like MLR applied to measured/CAMx NO_2 columns can identify and prioritize **areas of EI improvement**

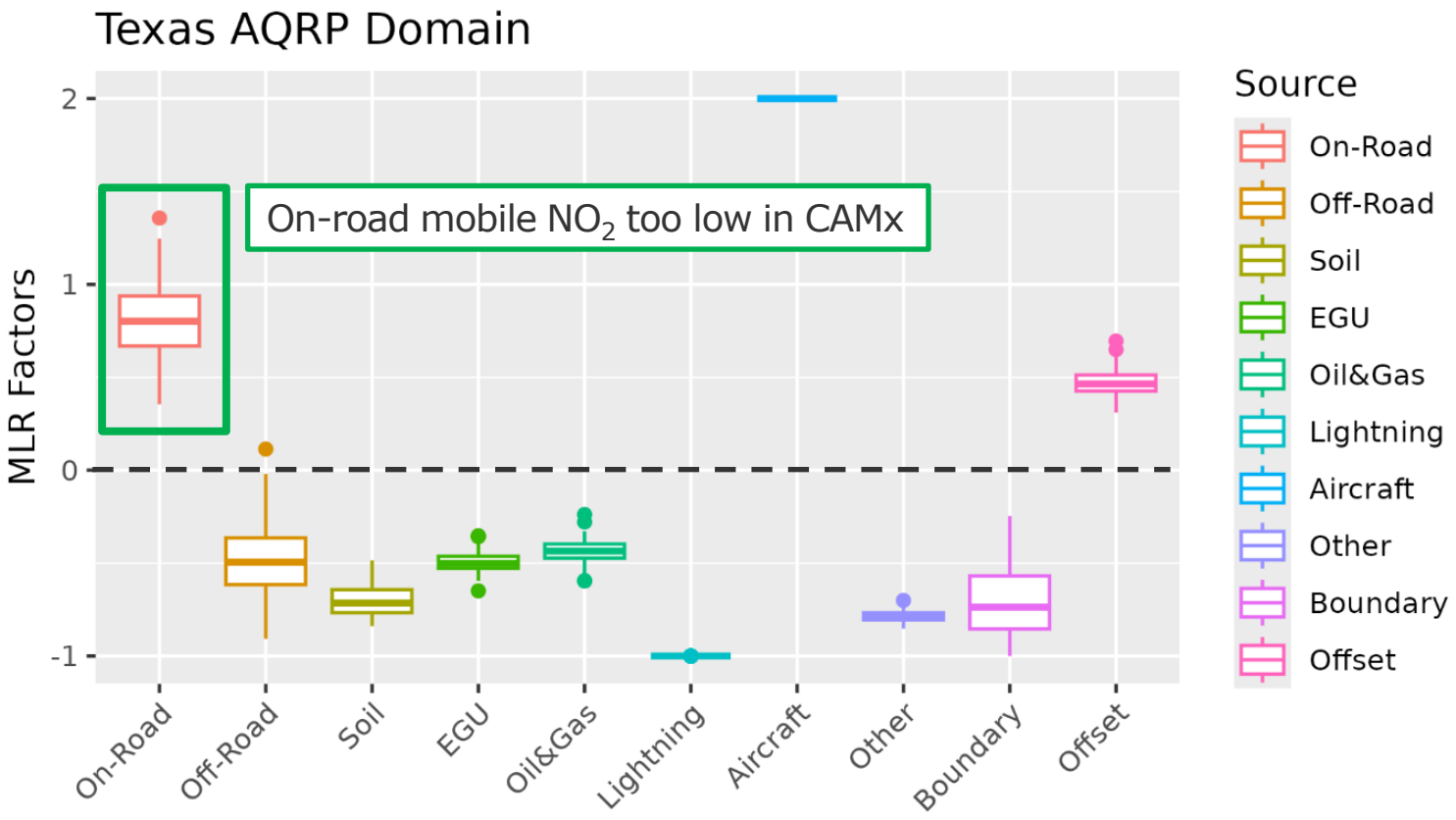


% of NOx EI in 444 m domain

Goldberg et al., 2024

Multiple Linear Regression (MLR) Models using TEMPO

- MLR seeks best match between TEMPO and tagged CAMx NO_2 Columns
- Zero value indicates no adjustment needed
  Positive: sector underestimated
  Negative: sector overestimated
- On-road mobile underestimated overall
  - Agrees with AQRP 22-023 results, but confidence lower
  - Larger underestimates in Dallas, better agreement in Houston and Central Texas
- Most other sectors overestimated
- MLR essentially zeroes out lightning NOx
  - Further investigation needed, but latest research suggests lower production efficiency (PE) than previously estimated
- MLR greatly increases aircraft emissions
  - TEMPO surface reflectivity issues may be present near airports
- Modeling period too short to provide robust evaluation of hourly results



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Summary and Conclusions

- Implemented ON hydrolysis and MEGAN v3.21 soil NOx updates in CAMx
- Improved near-surface ozone and NO_2 performance with revised MEGAN soil NOx updates
- TEMPO NO_2 10-20% larger than TROPOMI NO_2 in urban areas, likely due to TEMPO higher spatial resolution
- CAMx NO_2 broadly larger than TEMPO NO_2 in rural areas likely due to natural (LNOx and biogenic) sources
- CAMx NO_2 lower than TEMPO NO_2 in urban areas
- TEMPO NO_2 stays constant throughout late afternoon, while CAMx NO_2 increases sharply
- MLR analysis suggests on-road mobile emissions underestimated
    - LNOx and most other sectors overestimated
- Month-long modeling period not long enough for MLR to provide emissions estimates by hour

Recommendations

- Investigate further refinements to soil HONO and NO emissions and evaluate with TEMPO
  - Further adjustments could include updates to soil temperature and moisture, decay period for available soil N from fertilizer, N deposition half-life, soil N availability for HONO, and fertilizer lifetime (1 month?)
- Investigate refinements to lightning NOx and aircraft emissions
- Investigate temporal allocation and overall magnitude of on-road and off-road vehicle NOx emissions, particularly in Dallas
- Repeat satellite comparison with tagged CAMx NO_2 columns as improved TEMPO retrievals are made available
- Develop new CAMx modeling platform for one year or more to enable the use of CAMx *a priori* in the development of TEMPO NO_2 VCDs that remove the artifacts of the GEOS-CF *a priori* information

Questions?

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