Source-sector NOx emissions analysis with sub-kilometer scale airborne observations in Houston during TRACER-AQ

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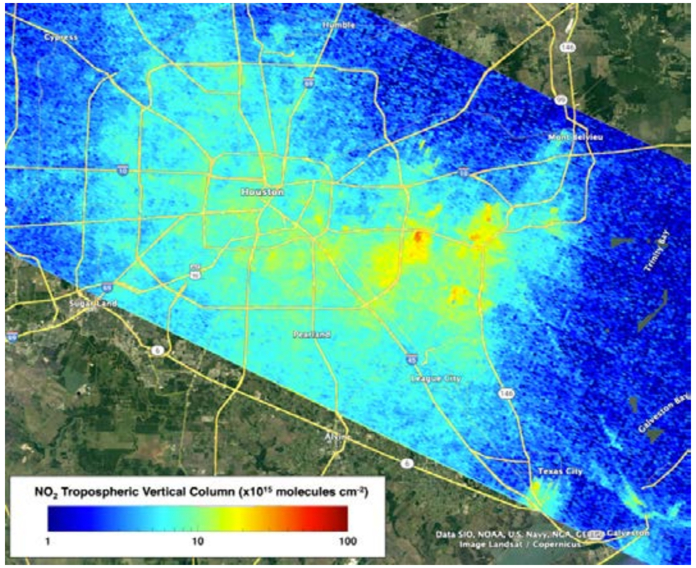
ESA: TROPOMI on the Sentinel 5 Precursor Satellite

This research presentation was supported by funding from the Texas Commission on Environmental Quality (TCEQ). The findings, opinions, or conclusions expressed do not necessarily represent those of the TCEQ.

Motivation of the Project

GCAS aircraft column NO_2 measurements from 28,000 ft



The high spatial resolution of GCAS (250 x 560 m^2) ***provides a unique ability to understand NO_2 sources***

Goal: To better understand the sector-by-sector NO_X emissions in the Houston metropolitan area during the TRACER-AQ September 2021 field campaign using a combination of:

- Ground measurements (i.e., Pandora spectrometers and CAMS monitors)
- Aircraft observations (i.e., GV aircraft with GCAS flying at 28,000 ft)
- Chemical transport models (i.e., WRF-CAMx with source apportionment)
- Satellite data (i.e., TROPOMI)

Methodology of project

Task 1. Simulate NO_2, HCHO, O_3 at 444 × 444 m^2 spatial resolution using WRF-CAMx

Task 2. Process the GCAS aircraft measurements – 10 days during September 2021

Task 3. Process the TROPOMI (satellite) NO_2 data during September 2021

Task 4a. Comparison of NO_2 (and HCHO) from aircraft, satellite, model to the "gold-standard" Pandora and CAMS monitors (when applicable)

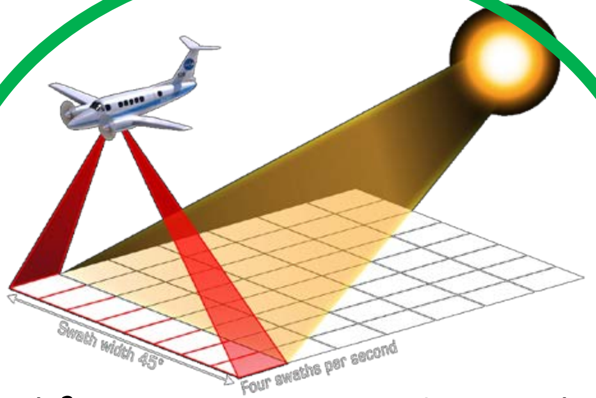
Task 4b. Comparison of NO_2 (and HCHO) between model, aircraft, and satellite

Task 5. Calculating NO_X from spatially continuous NO_2 airshed measurements

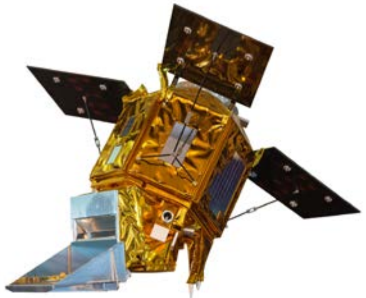
Task 6. Use of a regression model to estimate potential NO_X emission adjustments for individual sectors

Summary of conclusions

Comparison with Pandora column NO_2



(r^2=0.80 and NMB of +3.2%)

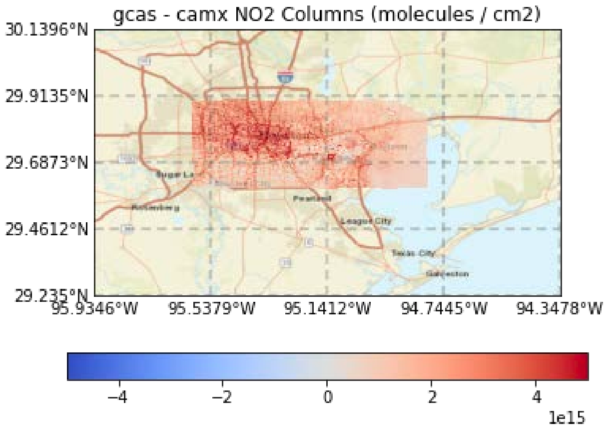


(r^2=0.62, and a small but important low bias: –11.2%)

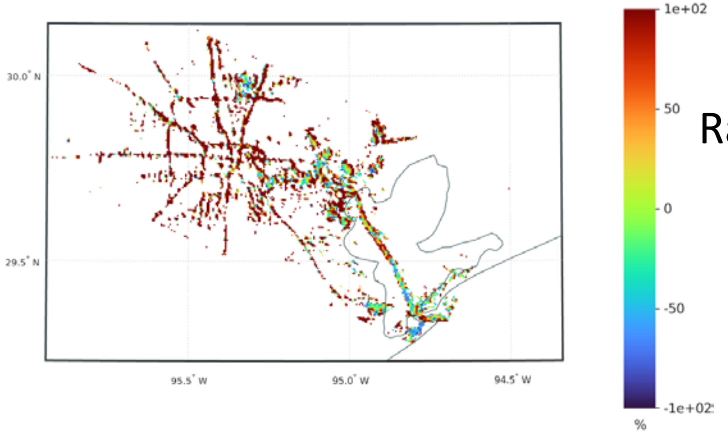
CAMx Ozone Particulates Toxics

(r^2=0.25, and a low bias: –20.2%)

Inferring NO_X emissions



CAMx NO_2 low bias worse in downtown

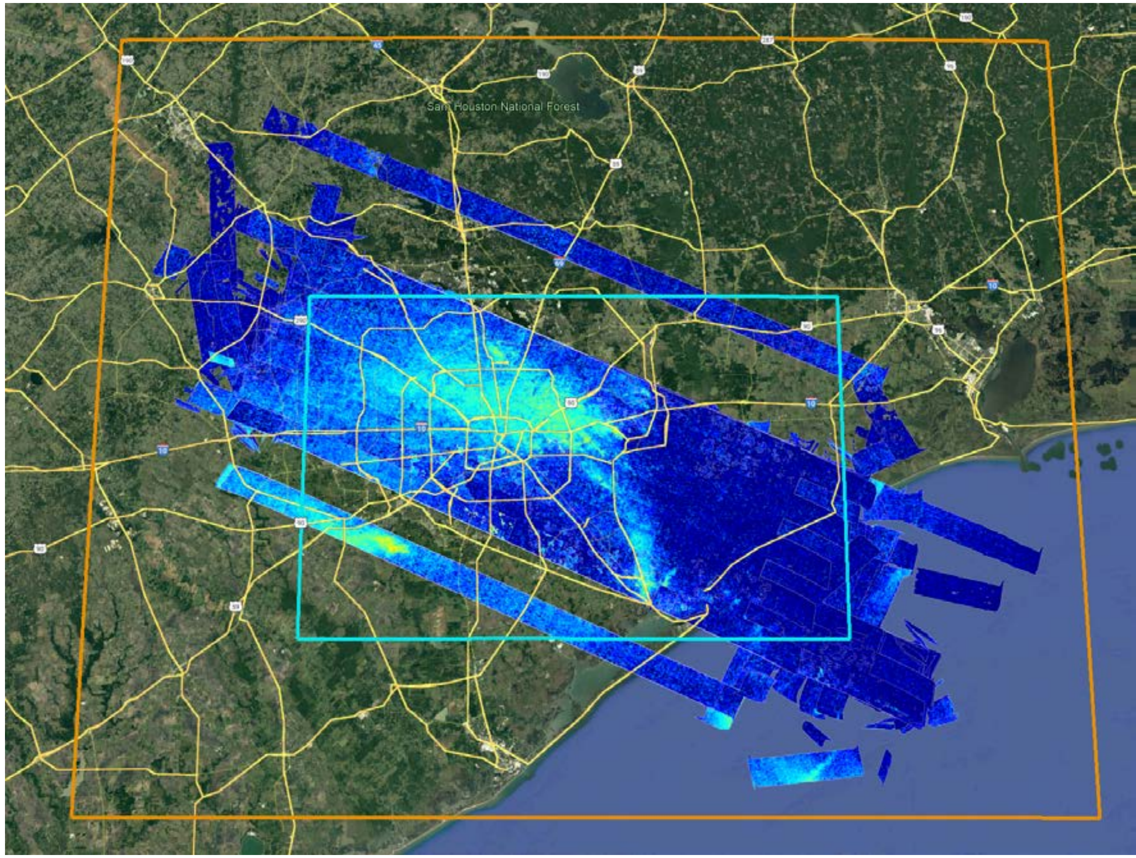


Ratio of NO_2 flux: GCAS / CAMx

CAMx NO_2 low bias worse near roadways

TRACER-AQ WRF and CAMx Model Configuration

- Use TCEQ 36/12/4 km 2019 SIP modeling platform as starting point
- Updates to TCEQ SIP modeling
  - WRF
    - New 36/12/4/1.333/0.444 km simulation
    - Physics options similar to TCEQ SIP modeling
    - <u>15-minute output frequency</u>
  - CAMx
    - Initial 36/12/4 km simulation based on TCEQ platform
    - Extracted boundary conditions from CAMx 4 km domain
    - 1.333/0.444 km domains over Houston to match resolution/extent of GCAS measurements
  - Emissions
    - Updated EGU emissions to use 2021 hourly CEMS data for top NOx emitters
    - 444 m resolution on-road and shipping emissions
    - Natural emissions driven by new WRF simulation
    - Re-processed 4 km emissions for other sectors to new grids



CAMx NO_2 Tagging and EGU NOx Emissions

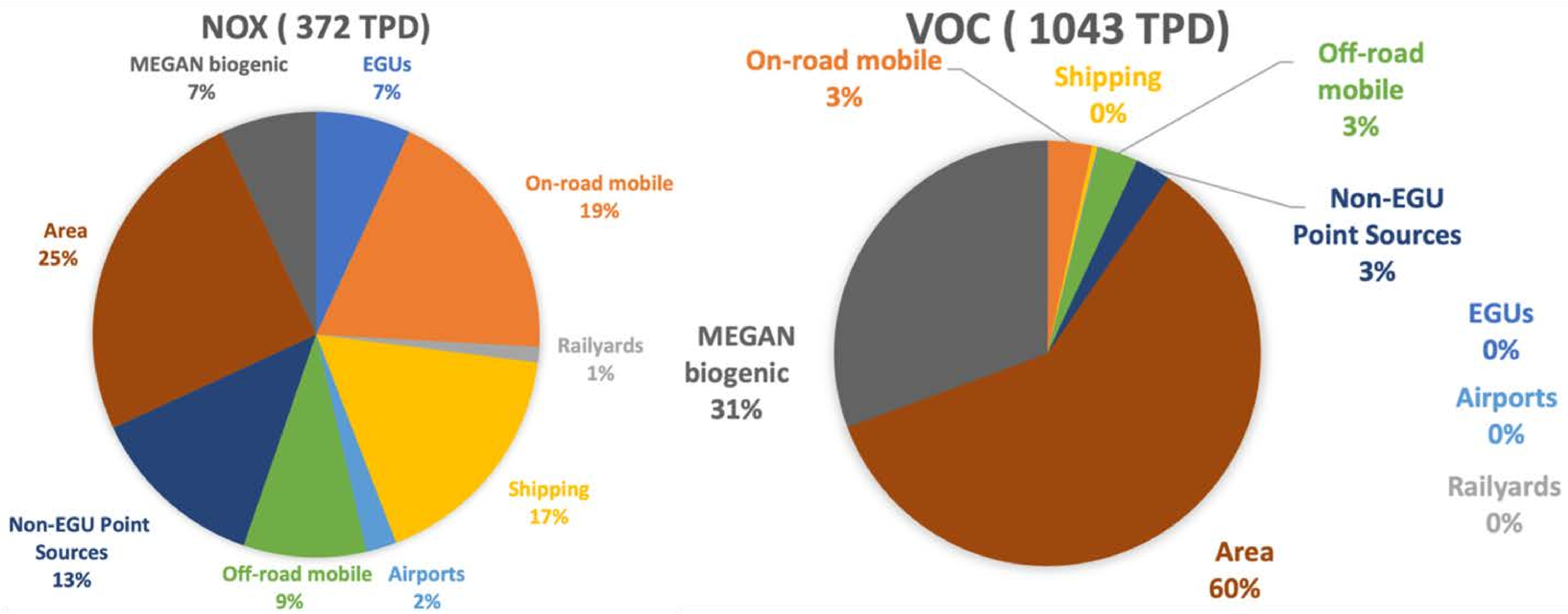
Number	Tagged Emissions Sector
1-9	EGUs
10	On-road mobile
11	Railyards
12	Shipping
13	KHOU airport
14	KIAH airport
15	Other

Station	NOx (tons/month)
W A Parish	570.7
Cedar Bayou	73.0
Pasadena Power Plant	34.7
Texas City Cogeneration	34.6
Odyssey Energy Altura Cogen, LLC	30.8
Deer Park Energy Center	27.4
South Houston Green Power Site	25.9
Air Liquide Bayport Complex	25.0
Channelview Cogeneration Facility	25.0

T H Wharton*
Greens Bayou*
Off-road mobile
Railway
Non-EGU point sources
Oil and Gas
MEGAN biogenic
Other Area

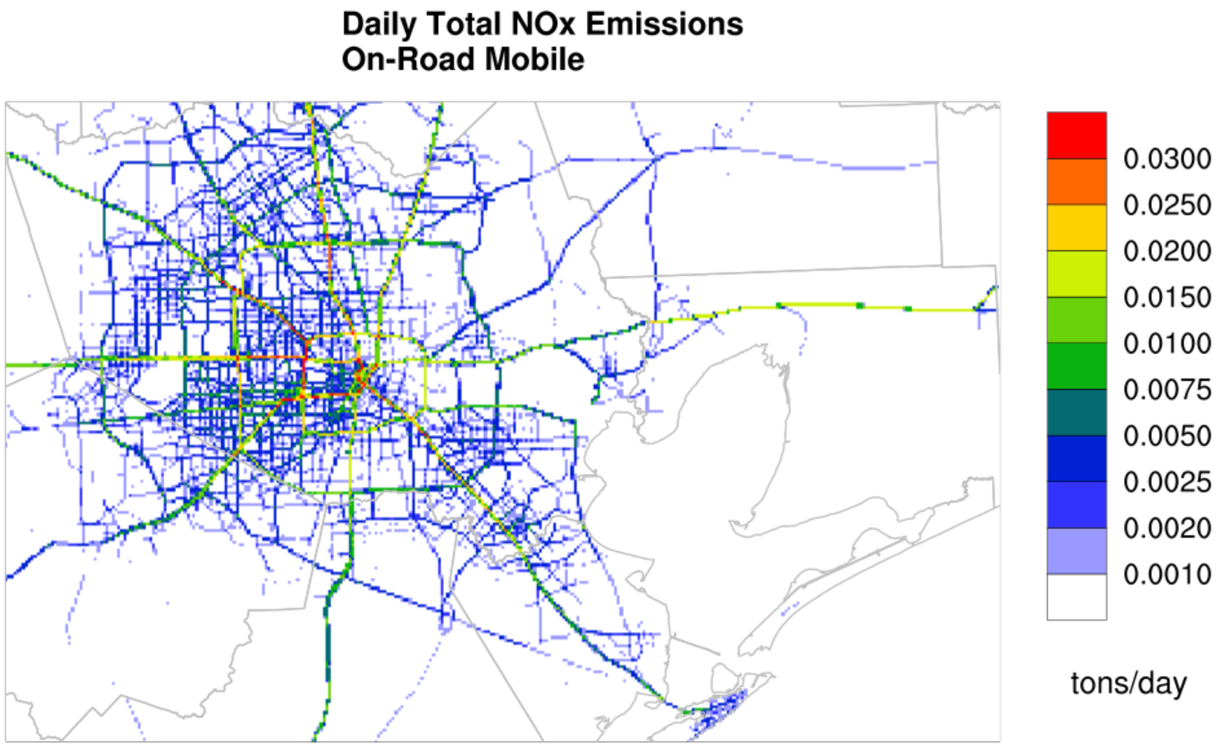
* Not tagged individually, but emissions from 2021 CEMS data

NOx and VOC Emissions Summary for 444 m Domain

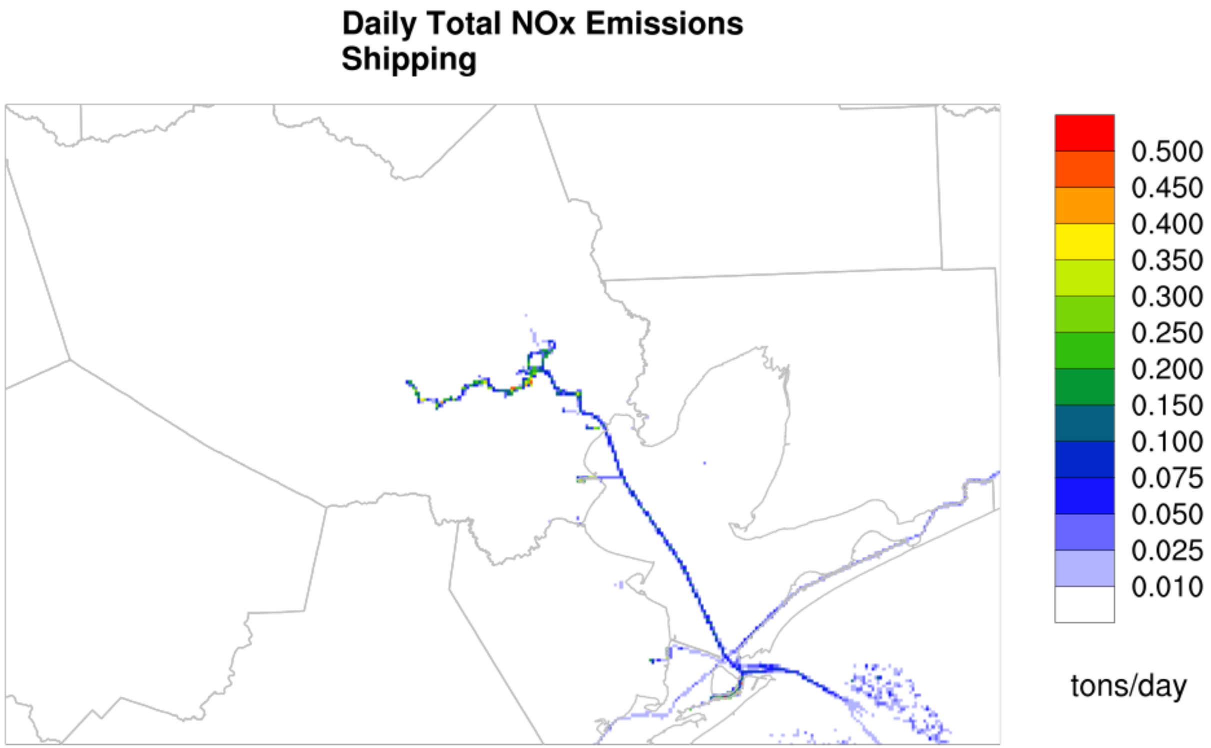


* Off-road mobile includes non-road and railway emissions

444 m On-Road Mobile and Shipping NOx Emissions



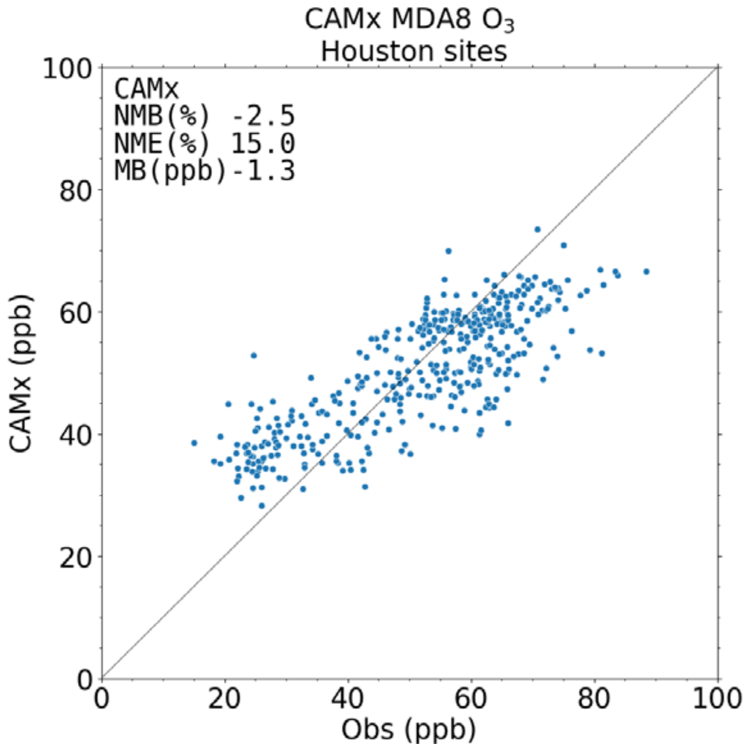
- Uses 2019 TCEQ on-road mobile link-based emissions
- Re-process links at 444 m resolution

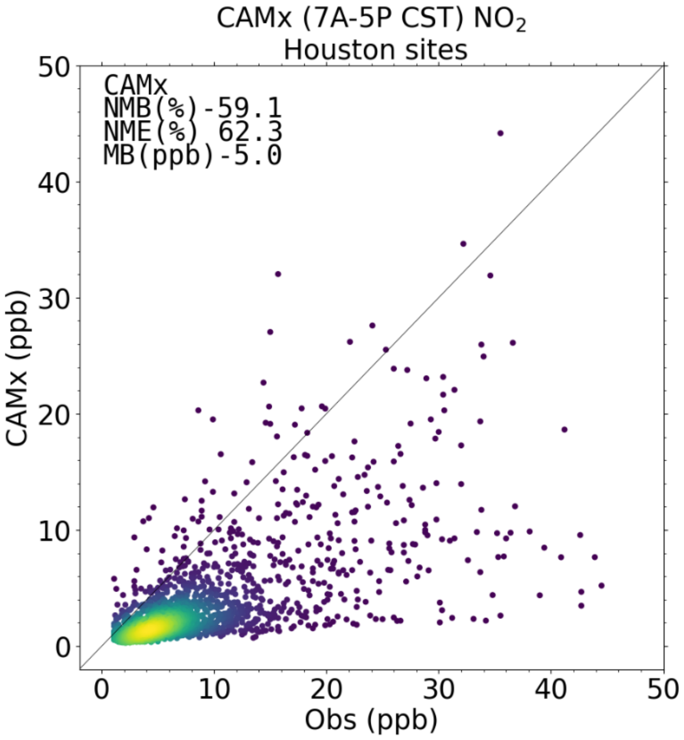


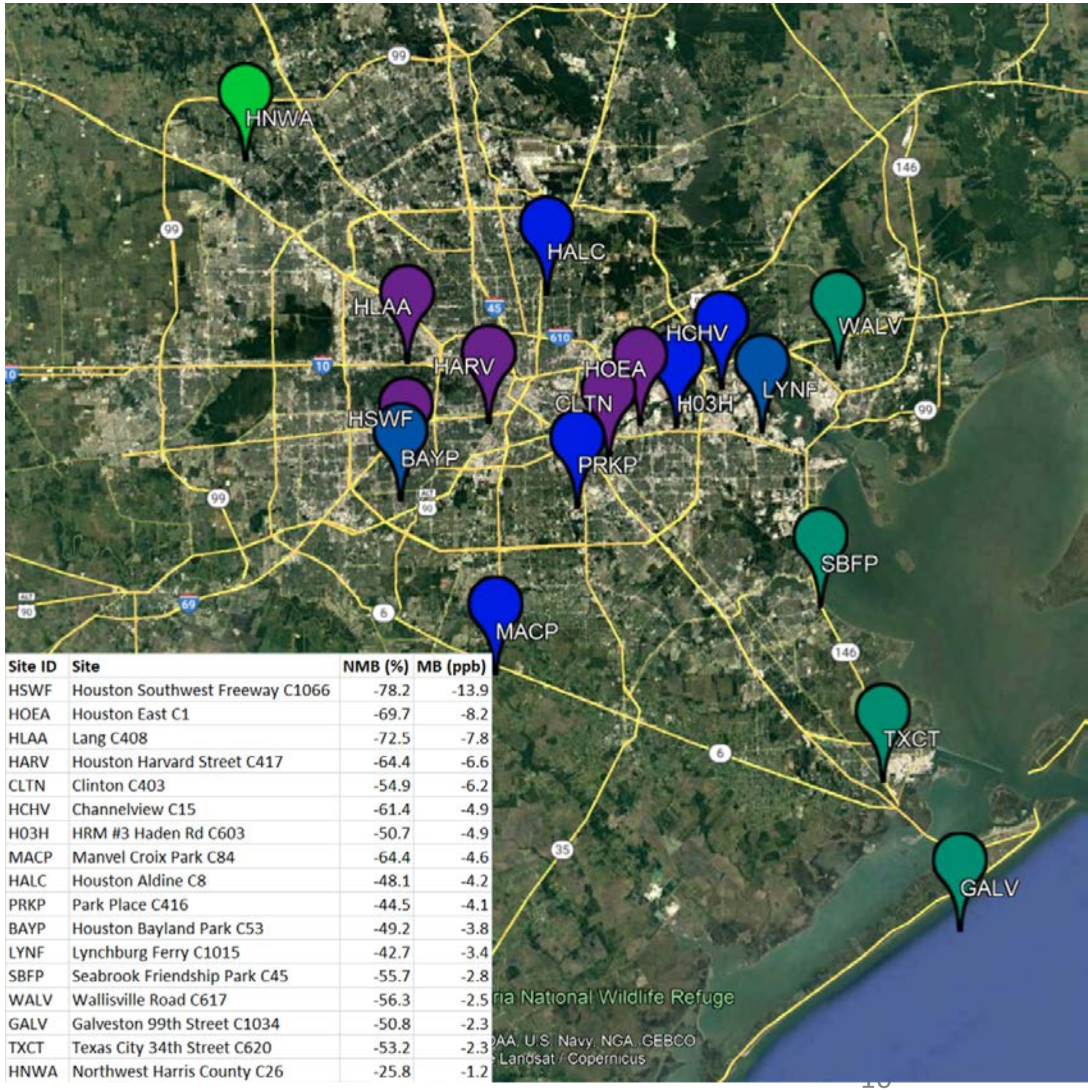
- Uses MARINE Emissions Resolver (MARINER) v2
- Vessel ID, location, operation: Automatic Identification System (AIS) data for 2021
- Vessel characteristics: IHS database

CAMx Ozone and NO_2 Model Performance at CAMS

- Overall excellent MDA8 ozone performance
  - NMB (± 5%) and NME (< 15%) very close to goal benchmark
- Overall low NO_2 bias, largest at higher observed NO_2 concentrations
- Smallest NO_2 bias at locations away from large emission sources
- Largest biases w/in Houston core near large emission sources
  - Houston SW Freeway CAMS ~50 m from roadway
  - 444 m resolution not sufficient to resolve near-roadway NO_2 here



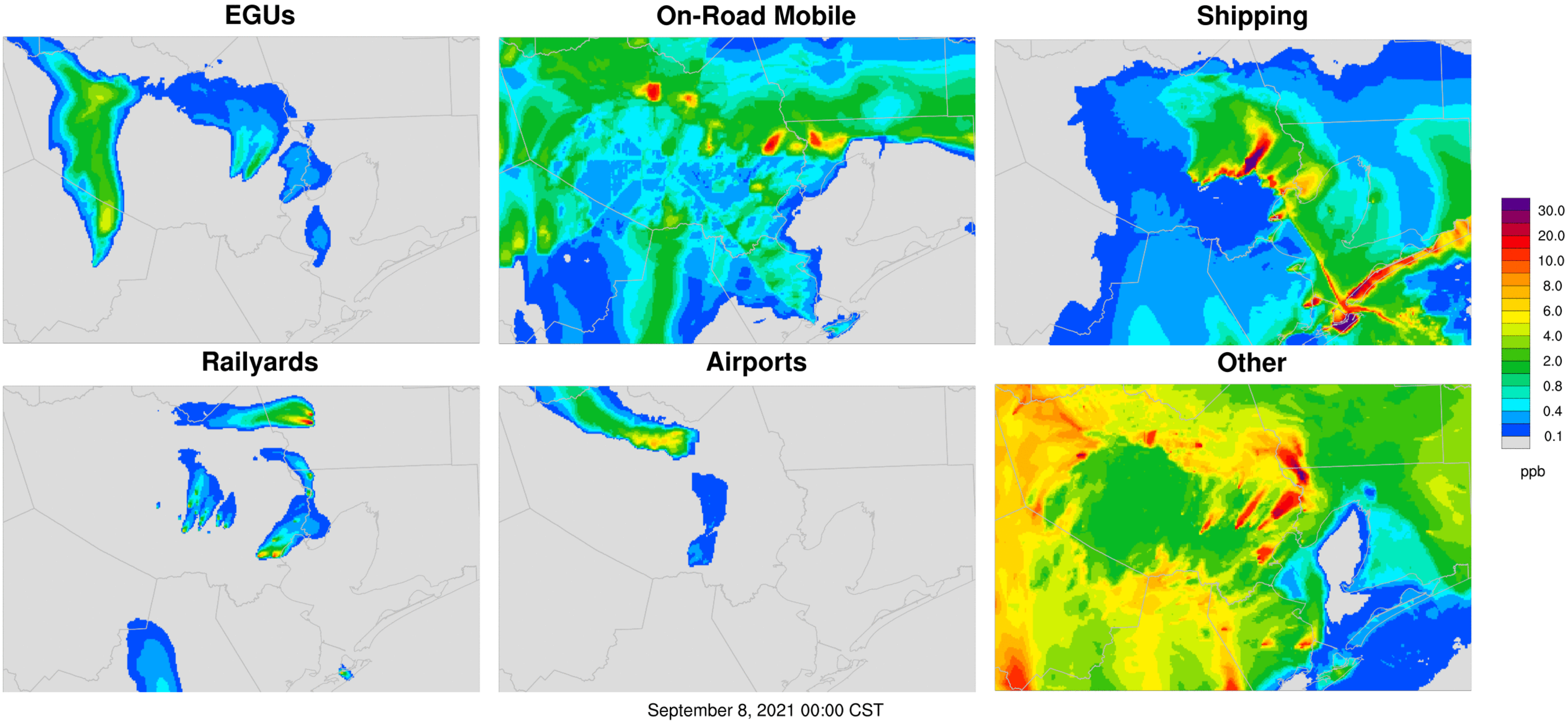




Site ID	Site	NMB (%)	MB (ppb)
HSWF	Houston Southwest Freeway C1066	-78.2	-13.9
HOEA	Houston East C1	-69.7	-8.2
HLAA	Lang C408	-72.5	-7.8
HARV	Houston Harvard Street C417	-64.4	-6.6
CLTN	Clinton C403	-54.9	-6.2
HCHV	Channelview C15	-61.4	-4.9
H03H	HRM #3 Haden Rd C603	-50.7	-4.9
MACP	Manvel Croix Park C84	-64.4	-4.6
HALC	Houston Aldine C8	-48.1	-4.2
PRKP	Park Place C416	-44.5	-4.1
BAYP	Houston Bayland Park C53	-49.2	-3.8
LYNF	Lynchburg Ferry C1015	-42.7	-3.4
SBFP	Seabrook Friendship Park C45	-55.7	-2.8
WALV	Wallisville Road C617	-56.3	-2.5
GALV	Galveston 99th Street C1034	-50.8	-2.3
TXCT	Texas City 34th Street C620	-53.2	-2.3
HNWA	Northwest Harris County C26	-25.8	-1.2

*Emery et al., 2017

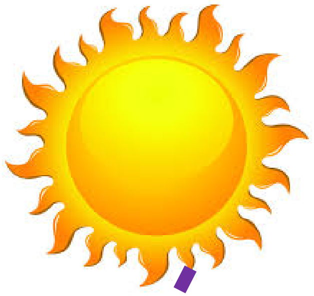
Hourly Tagged NO_2 Contributions – Sep 8, 2021



How is remotely-based NO_2 "measured"?

1. Radiances measured in the 400-450 nm visible wavelength region (indigo) are used to create a <u>*total slant column*</u> between detector and ground

2. Use an "air mass factor" – partially derived from a model – to convert slant column to vertical column



passive spectrometer

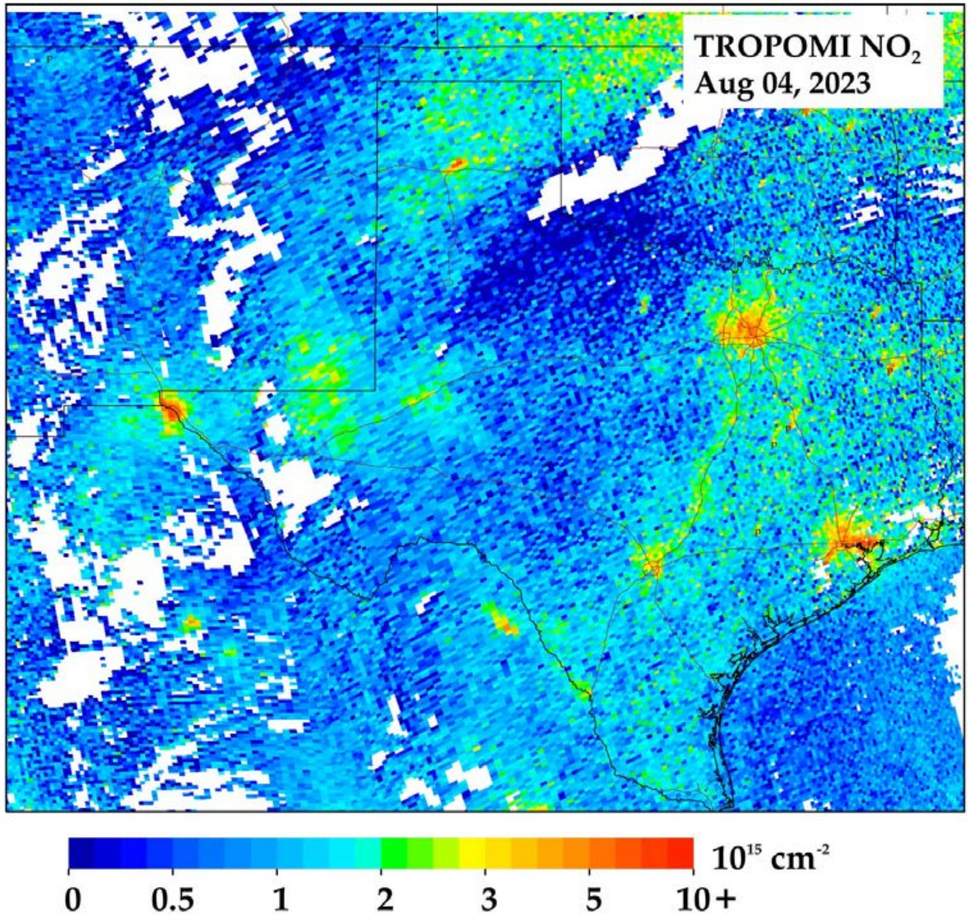
For more info: [Levelt et al., 2006]

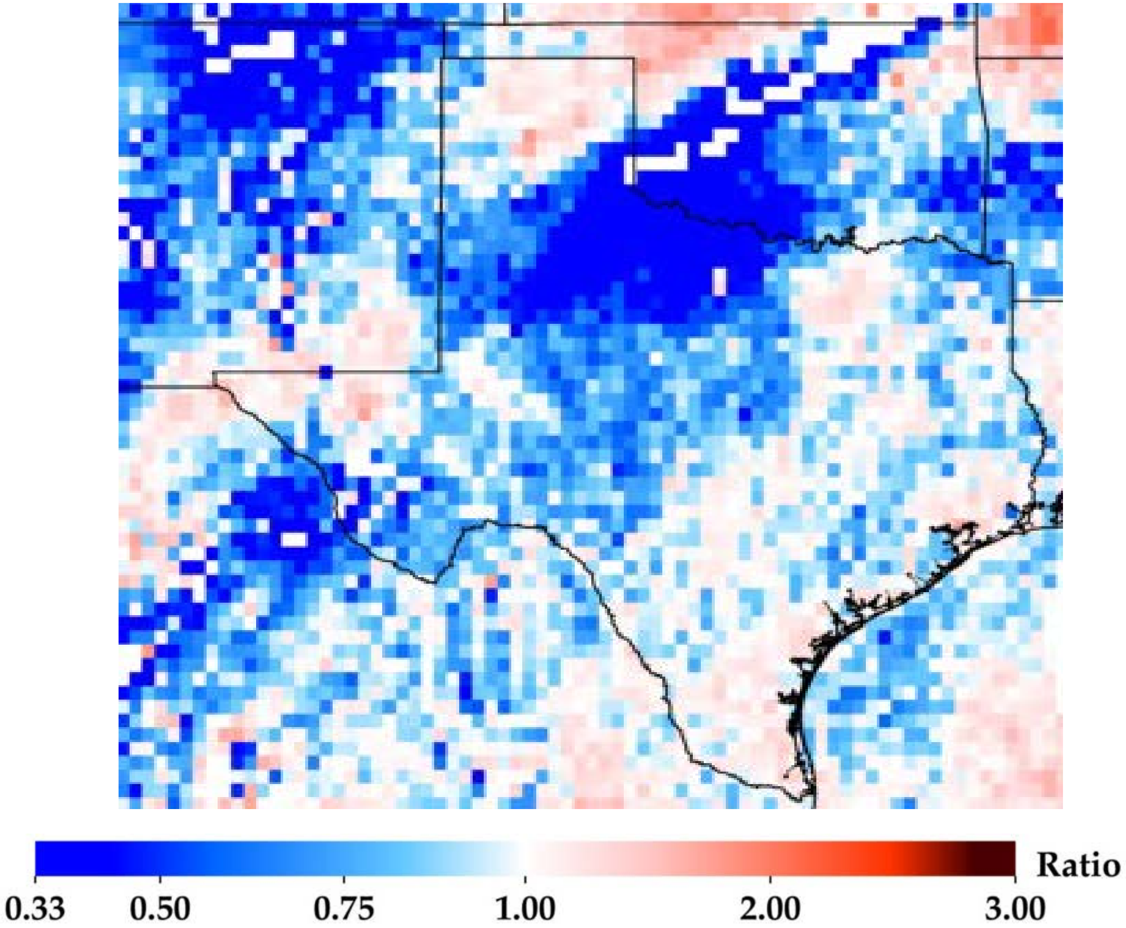
W.A. Parish Power Plant

Houston Skyline

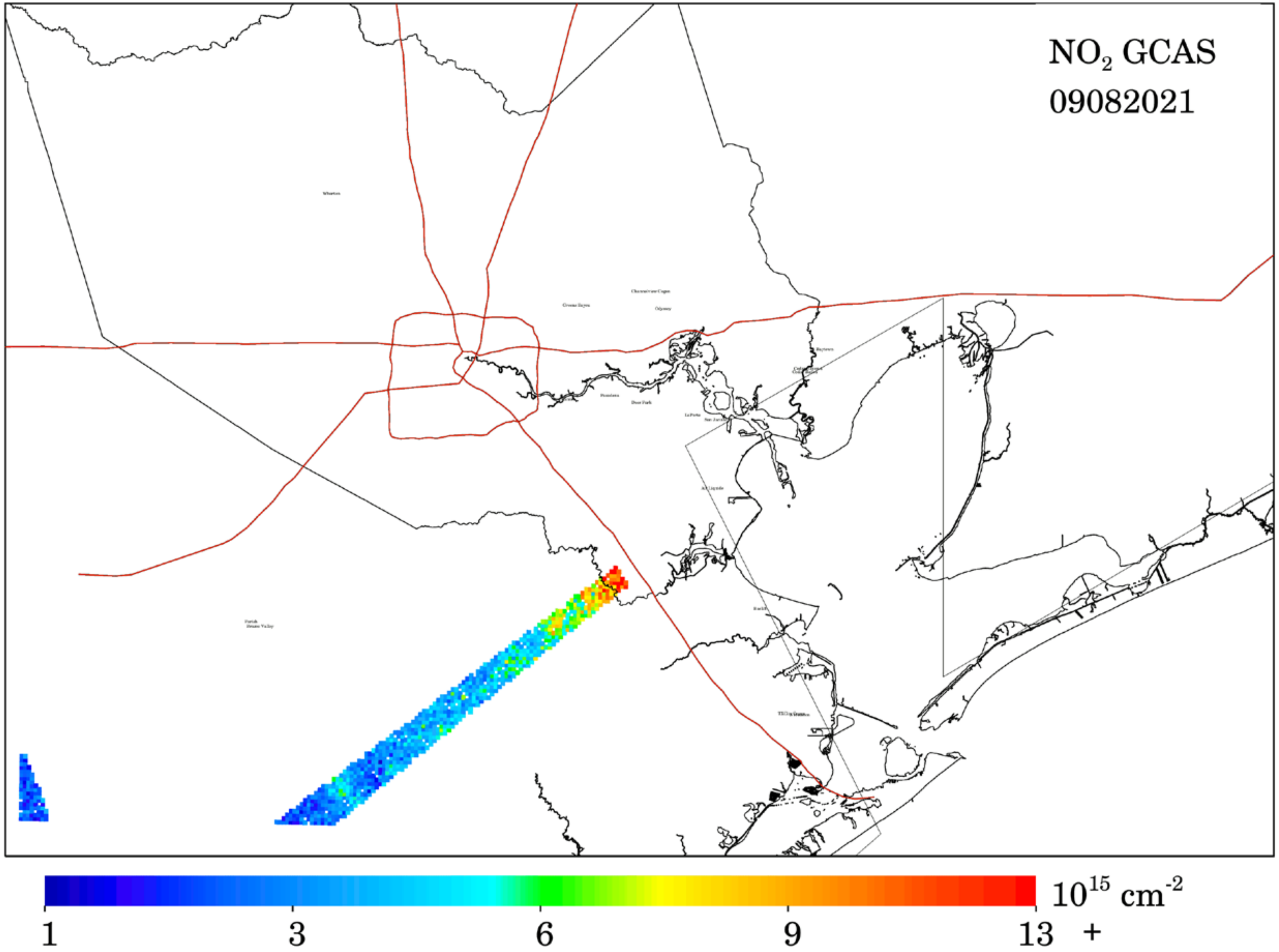
Near-real-time images of TROPOMI NO_2

tropomino2.us



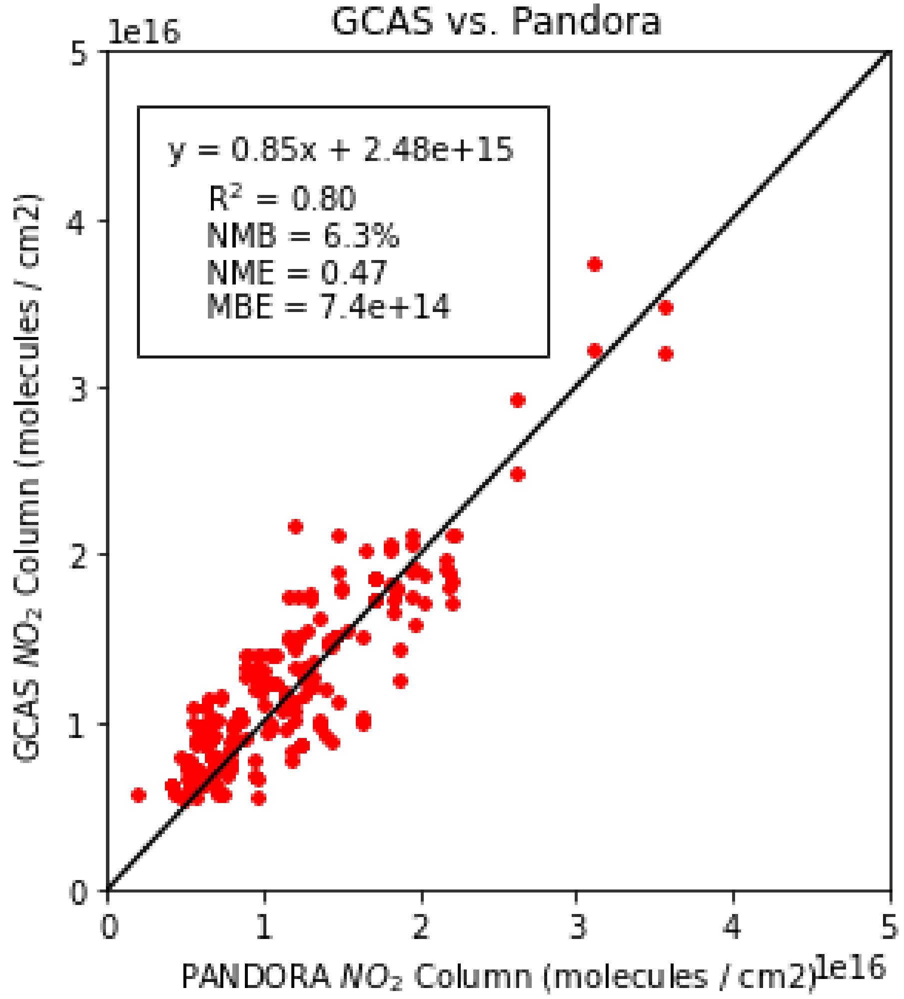


GCAS column NO_2 data from September 8, 2021

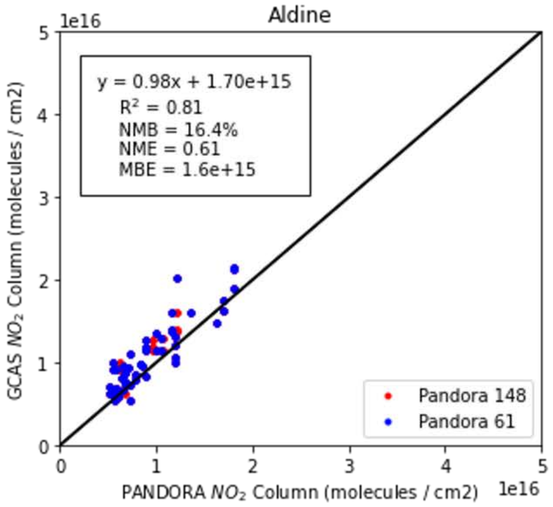


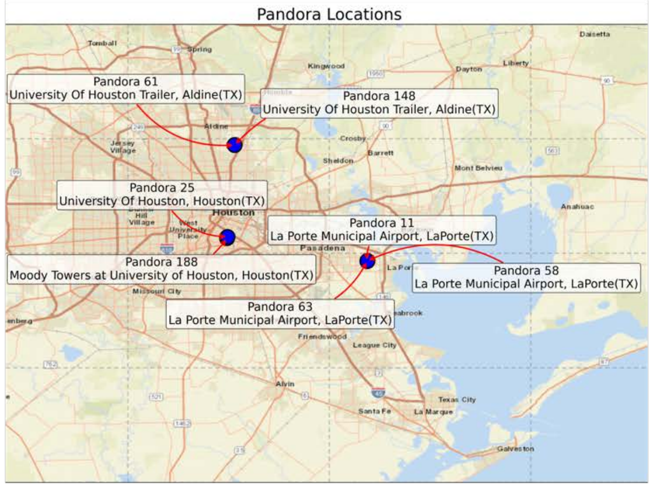
How does GCAS aircraft compare to Pandora? Matches Pandora with excellent correlation

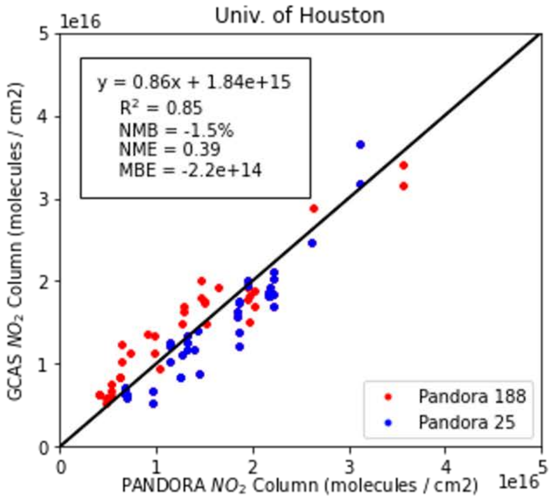
- Pandora uses fewer assumptions and assumed to be closest to a “reference”

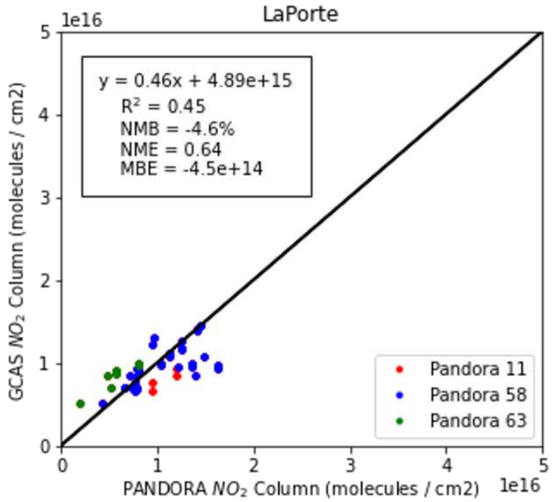


How does GCAS compare to Pandora?
Matches Pandora with excellent correlation









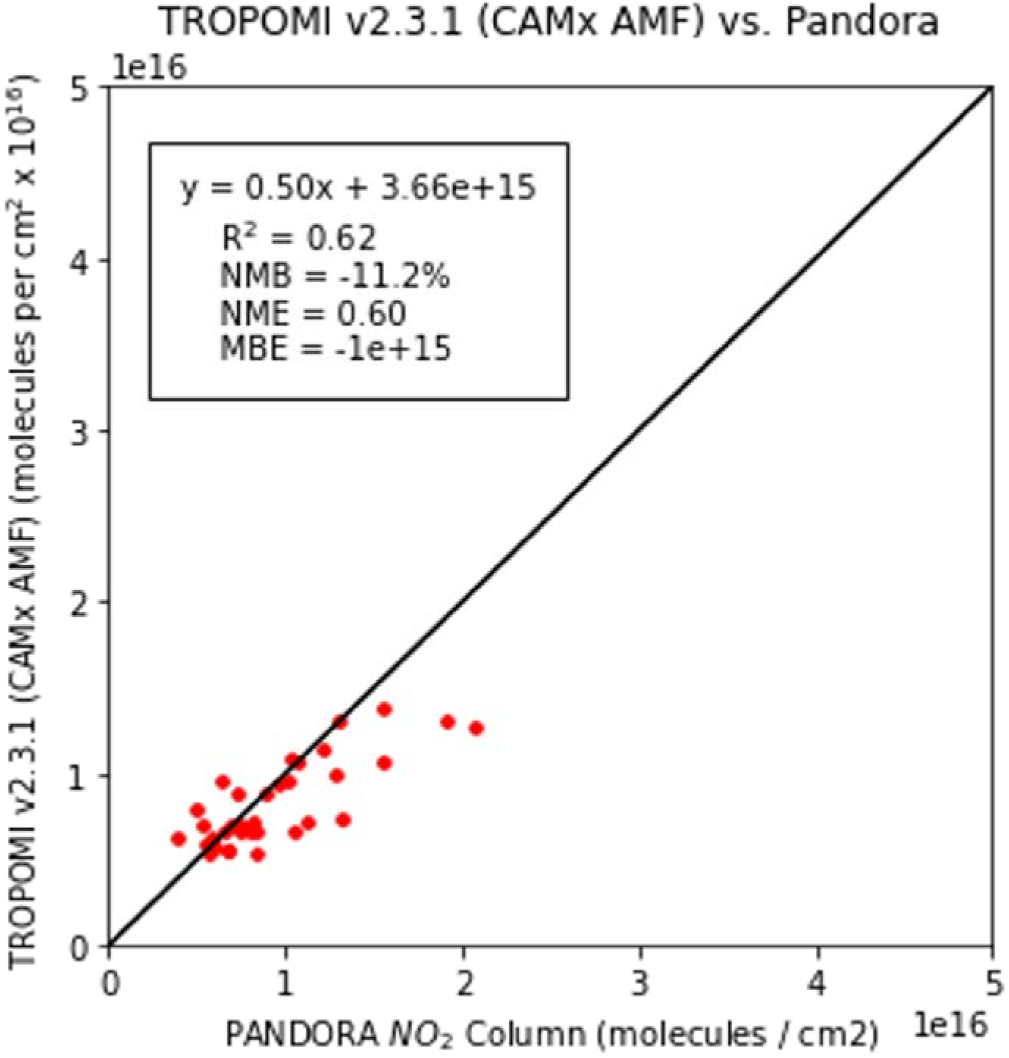
3 Pandora sites during TRACER-AQ: Aldine, U. Houston & LaPorte

Excellent correlation at the Aldine & University of Houston sites

Pandora 25 located at U. Houston situated on the ground, while Pandora 188 on top of the building

TROPOMI column NO_2 data

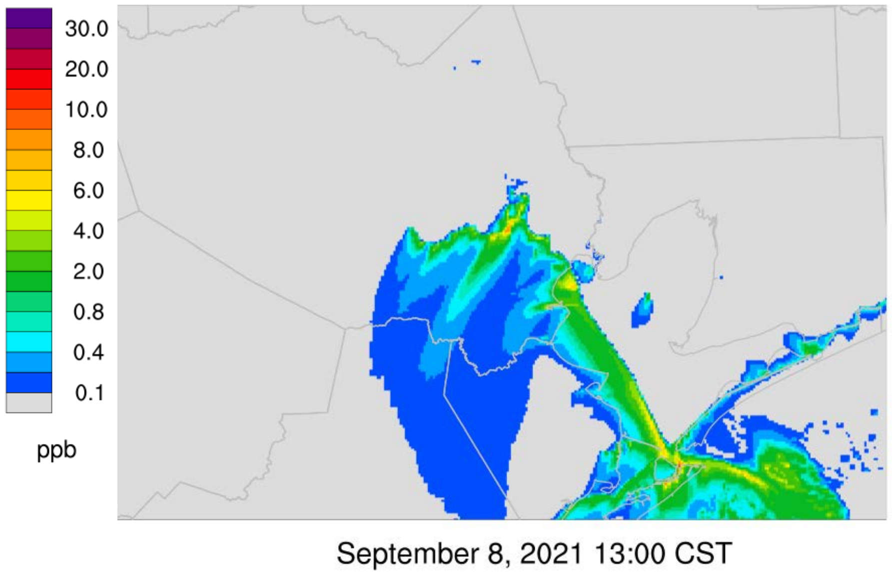
How does TROPOMI compare to Pandora? Appears to have a low bias but good correlation

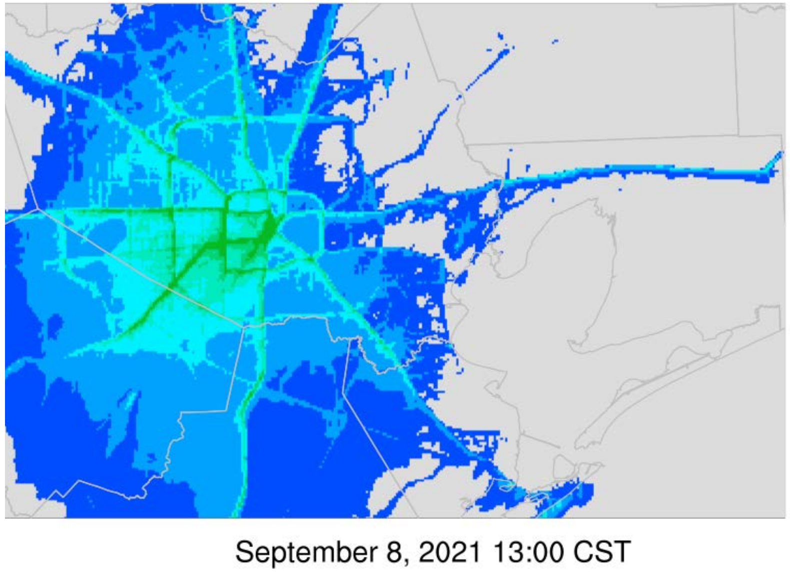


Comparison of CAMx against TROPOMI – Sep 8, 2021

- Houston has complex NO_2 emission signatures at finer scale than TROPOMI can resolve

Shipping NO_2 Contributions (ppb) **On-Road Mobile NO_2 Contributions (ppb)** **TROPOMI NO_2 Columns (molec/cm^2)**



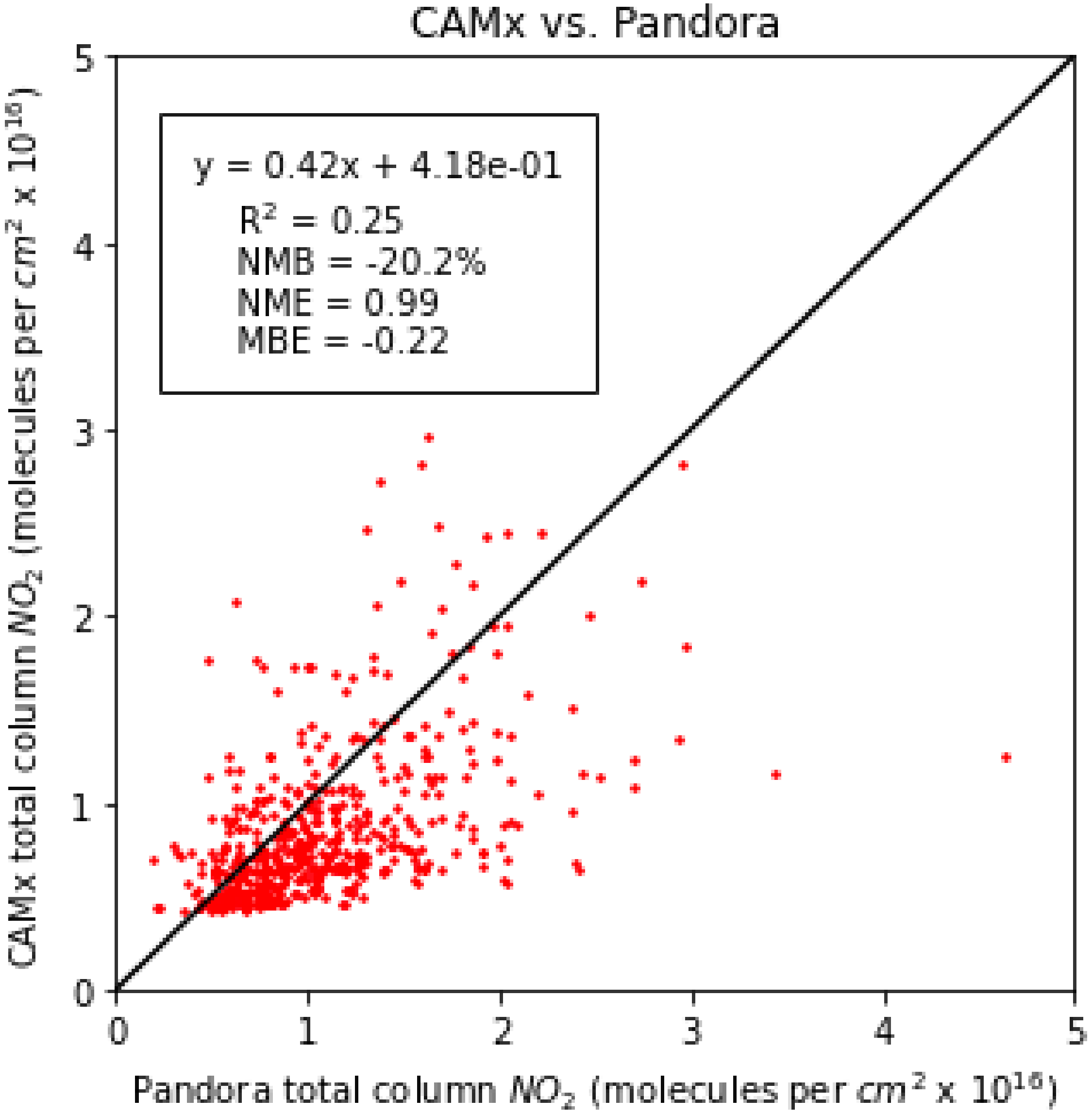


Performance of CAMx NO_2 column vs Pandora: Low bias and relatively low correlation

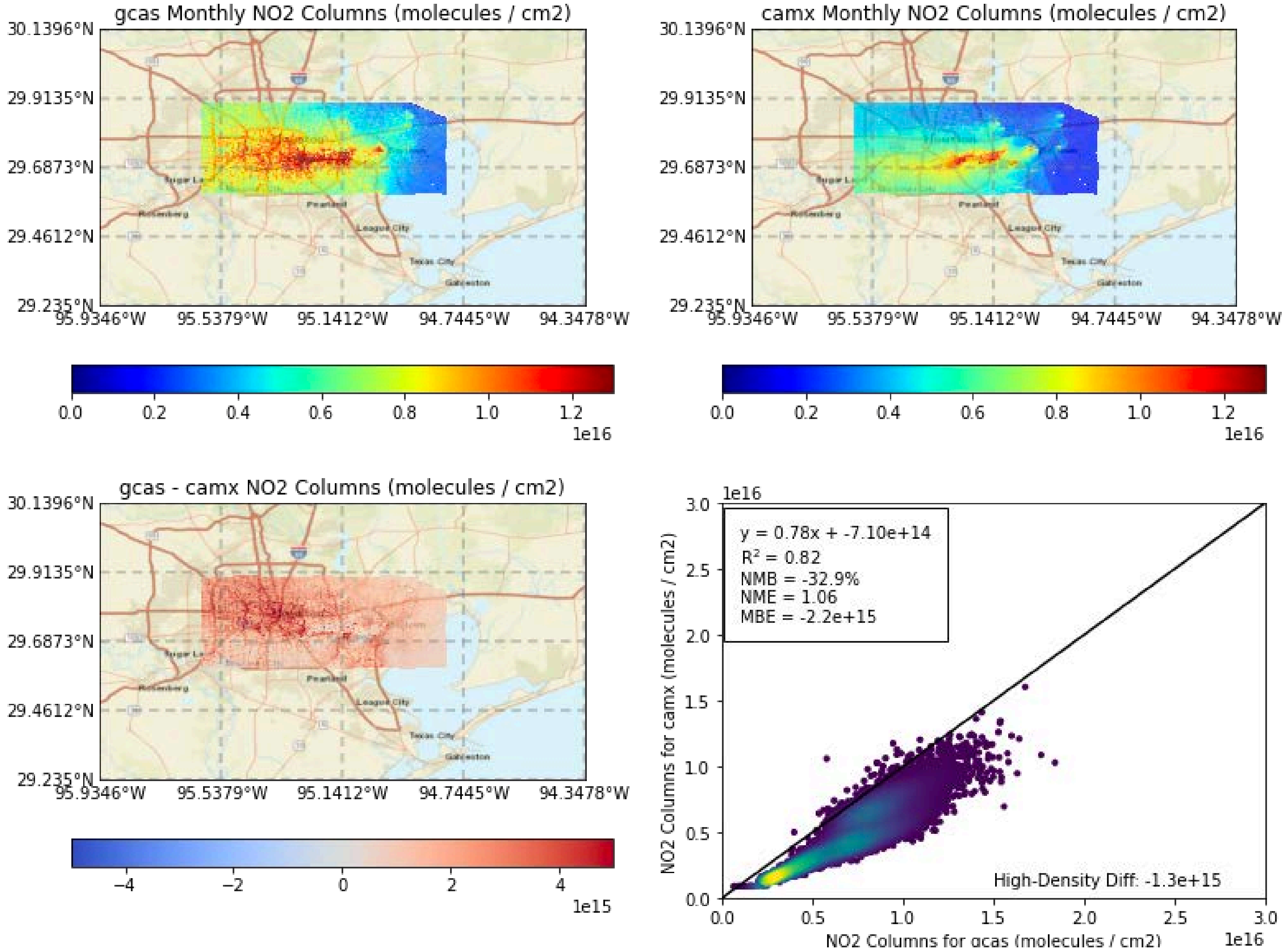
Low correlation ($r^2 = 0.25$) and a NMB of –20.2%.

Low correlation could be related to the difficulty in simulating wind direction and the Gulf/Bay breeze

Not shown: NMB worse on weekdays (7 days) than weekends (3 days)



CAMx has low NO_2 bias in downtown Houston



<u>GCAS vs. CAMx:</u>

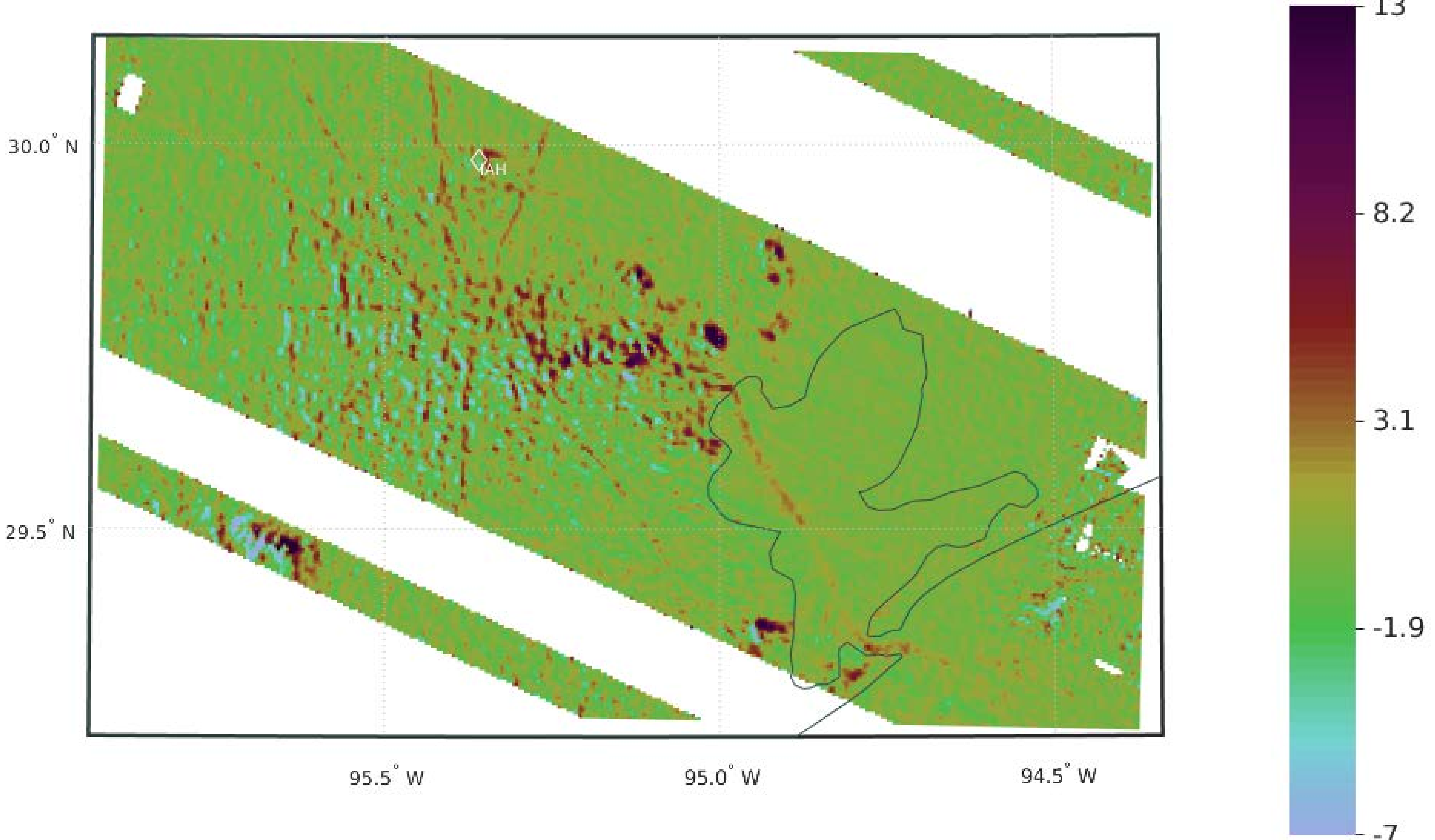
Worse low bias (–32.9%) than the CAMx vs. Pandora intercomparison (–20.2%)

But the correlation between CAMx and GCAS was very strong ($r^2 = 0.82$)

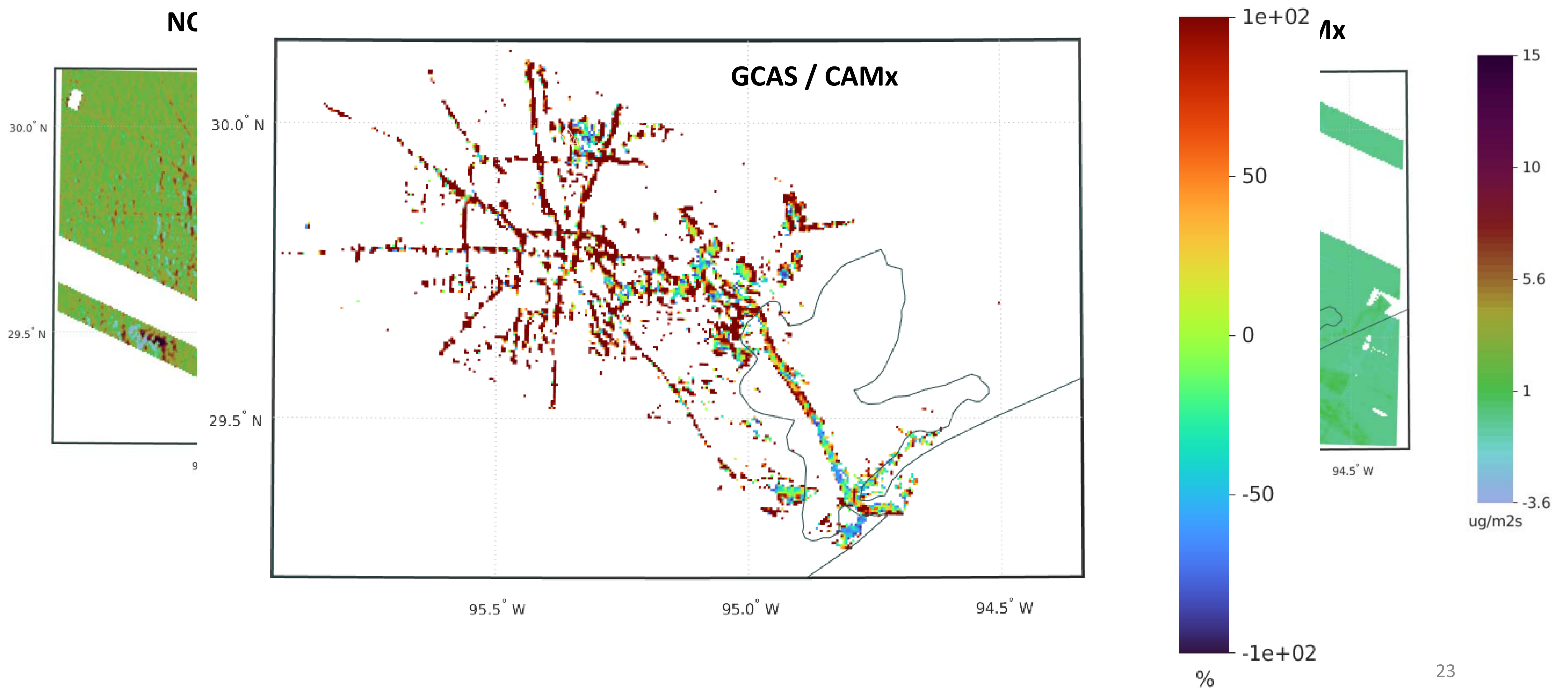
Largest difference between CAMx and GCAS is in the downtown section of Houston

Deriving NOx emissions in the metropolitan area Implicating missing on-road NO_2 sources

NO_2 fluxes as derived from GCAS



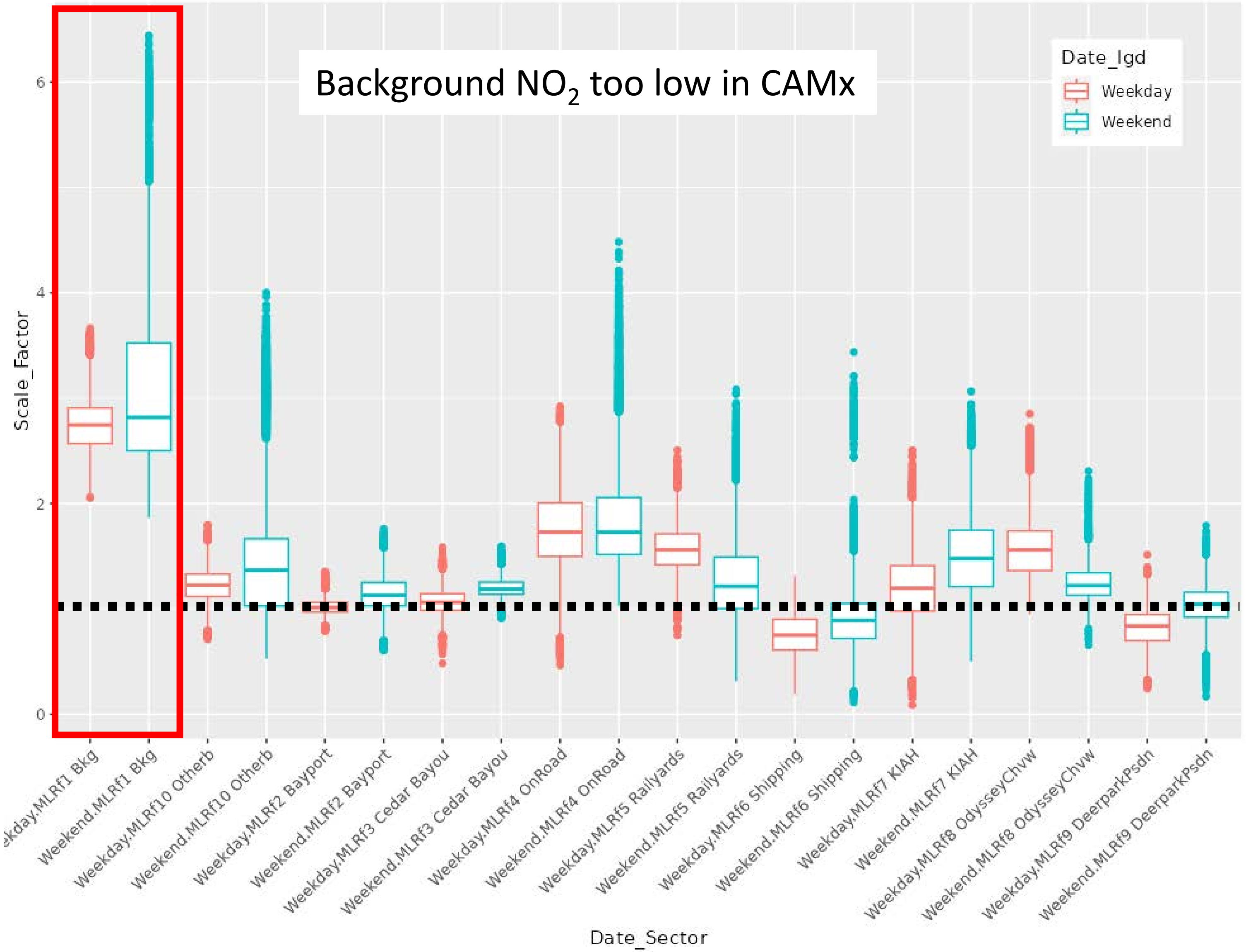
Deriving NOx emissions in the metropolitan area Implicating missing on-road NO_2 sources



Using a MLR model to estimate potential sector discrepancies: Background NO_2 in CAMx is too low

Figure showing **scale factor** needed for CAMx tagged NO_2 in order to replicate the GCAS NO_2

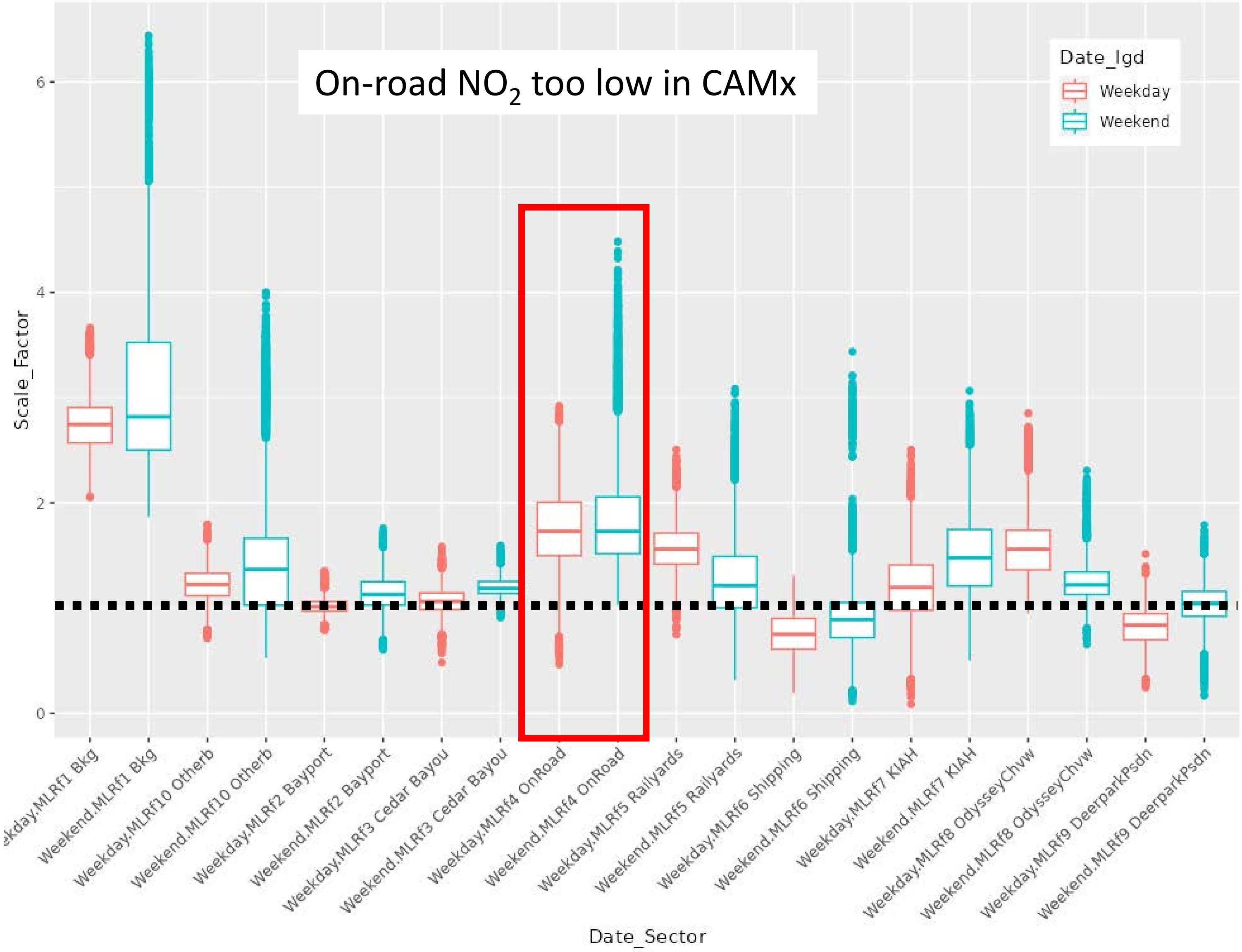
- Near 1 → no change needed
- >>1 → NO_2 needs to increase; NOx underestimate
- <<1 → NO_2 needs to decrease; NOx overestimate



Using a MLR model to estimate potential sector discrepancies: On-road NO_X emissions may be too low by factor of 1.72

Figure showing **scale factor** needed for CAMx tagged NO_2 in order to replicate the GCAS NO_2

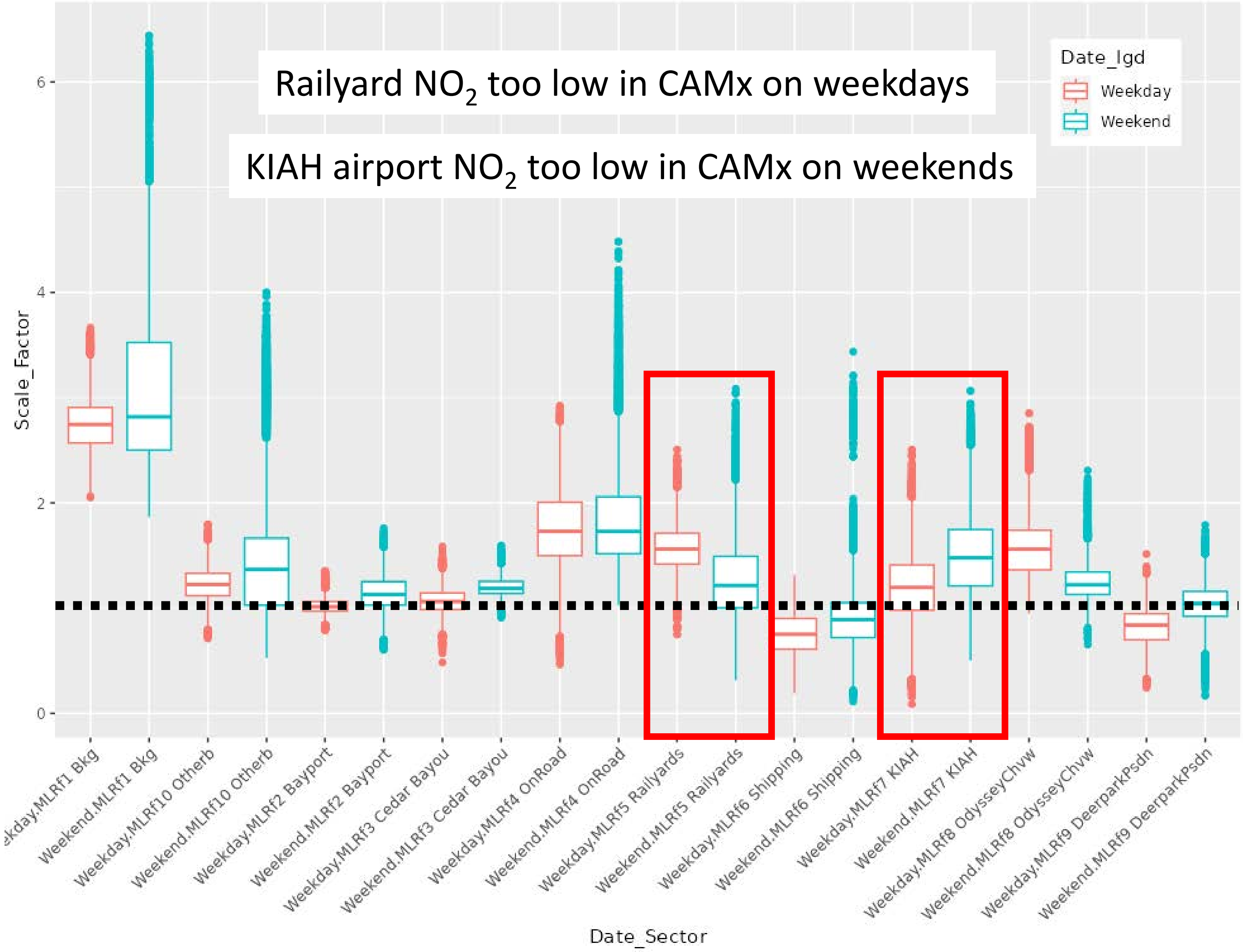
- Near 1 → no change needed
- >>1 → NO_2 needs to increase; NOx underestimate
- <<1 → NO_2 needs to decrease; NOx overestimate



Using a MLR model to estimate potential sector discrepancies: Railyard and airport NO_X emissions may be too low by factor of 1.5

Figure showing **scale factor** needed for CAMx tagged NO_2 in order to replicate the GCAS NO_2

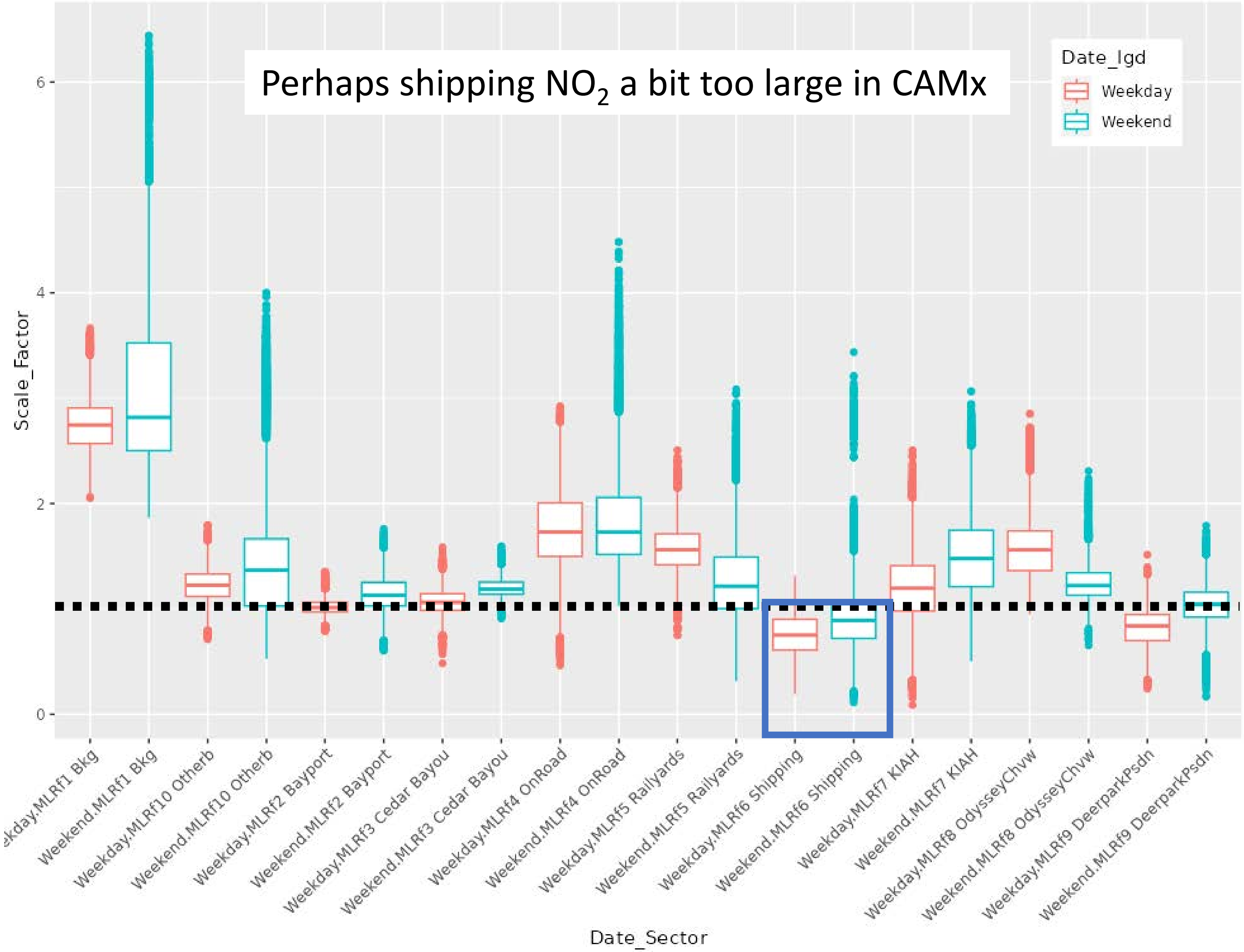
- Near 1 → no change needed
- >>1 → NO_2 needs to increase; NOx underestimate
- <<1 → NO_2 needs to decrease; NOx overestimate



Using a MLR model to estimate potential sector discrepancies: Shipping NO_X emissions may have a slight NO_X overestimate

Figure showing **scale factor** needed for CAMx tagged NO_2 in order to replicate the GCAS NO_2

- Near 1 → no change needed
- >>1 → NO_2 needs to increase; NOx underestimate
- <<1 → NO_2 needs to decrease; NOx overestimate



Conclusions (Part 1)

Task 1:

- CAMx (444 × 444 m^2) achieves the goal benchmark for MDA8 ozone but has a low bias for NO_2 at CAMS monitors (NMB of –59.1%), which we partially attribute to the difficulty of capturing hourly and near-road variability.

Task 2:

- GCAS aircraft-based measurements acquired fine-scale structure of urban NO_2 (250 × 560 m^2).
- GCAS column NO_2 has excellent agreement with Pandora NO_2 (r^2=0.81 and NMB of +6.3%)

Task 3:

- Satellite NO_2 has great correlation with Pandora measurements (r^2=0.62), but a low bias (–11.7%).

Conclusions (Part 2)

Task 4:

- CAMx versus Pandora column NO_2 showed a low bias in CAMx (–20.2%)
- CAMx versus GCAS column NO_2 showed larger CAMx NO_2 underestimates (–27%) and especially in downtown Houston.

Task 6:

- MLR suggests that NO_X from on-road mobile, railyard (weekday), and airport (weekend) may be underestimated.

Task 5:

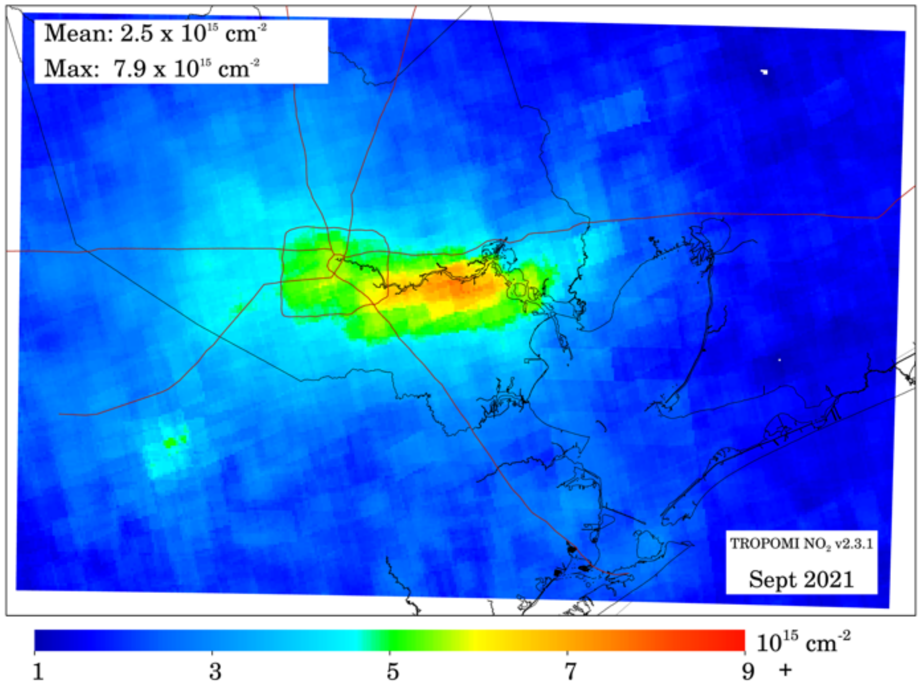
- The Flux Divergence method was able to distinguish the linear shape of major highways, many of the large point sources, and the Galveston Bay ship track.
- Point source NOx emissions matched reasonably well with the exception of the Baytown area on September 8, 2021 (modelled NOx too low)

Future recommendations

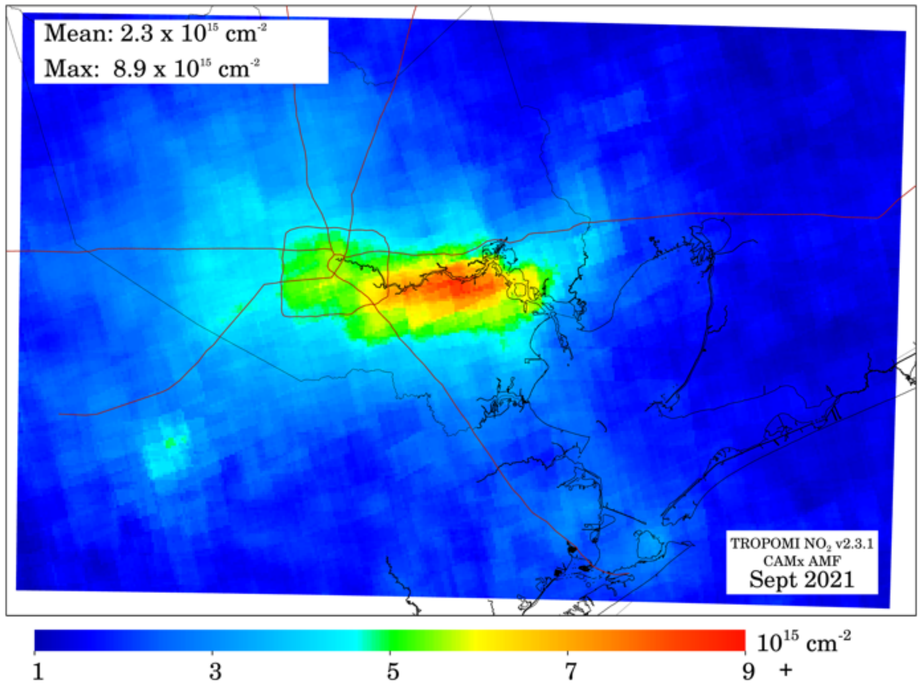
- Investigate biases found for on-road and port (rail, airport, shipping) NOx emissions in a new CAMx simulation, while also accounting for the different weekday/weekend biases.
    - Is there better agreement between observations and CAMx when NO_X emissions are increased?
- Investigating the cause of the low bias in TROPOMI over Houston.
    - Related to pixel size or something else? How does the NASA algorithm perform? Does TEMPO observe the same patterns as GCAS and TROPOMI?
- Use TROPOMI to investigate NO_2 over longer timeframes.
    - Are similar patterns seen? Are spatial NO_2 trends consistent with the NO_X inventory trends?
- More upper tropospheric measurements and measurements outside of urban locations are needed to better constrain GCAS and TROPOMI in the less polluted areas of Texas.
    - Performance of GCAS outside of urban areas is largely unvalidated. AEROMMA 2023 campaign will help.
- Further analysis of HCHO
    - Do anthropogenic VOC emissions need to be increased? If VOC emissions need to be modified, how does this affect the NO_2 lifetime, model NO_2 intercomparison, and O_3 model performance?

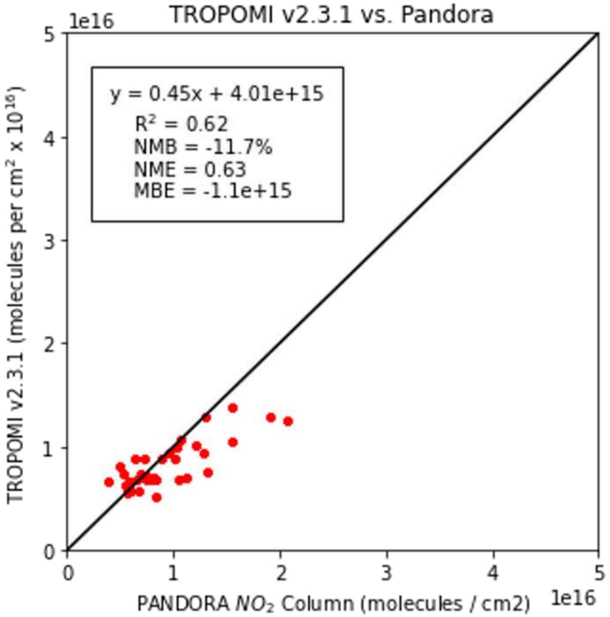
EXTRA Figures

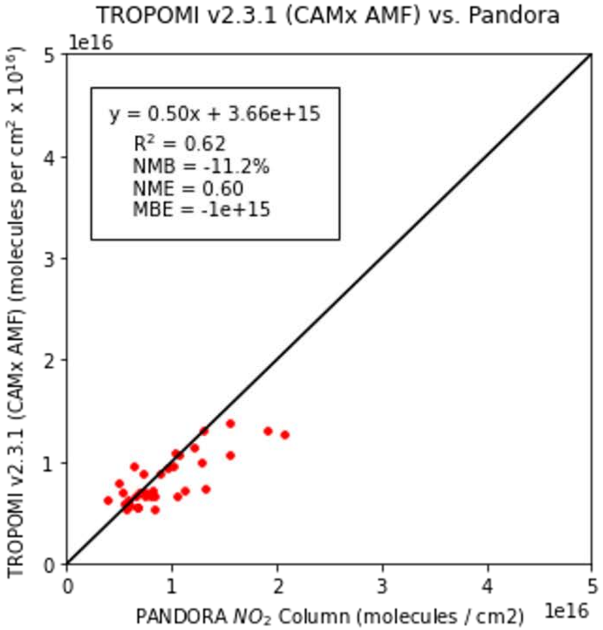
TROPOMI NO_2 v2.3.1

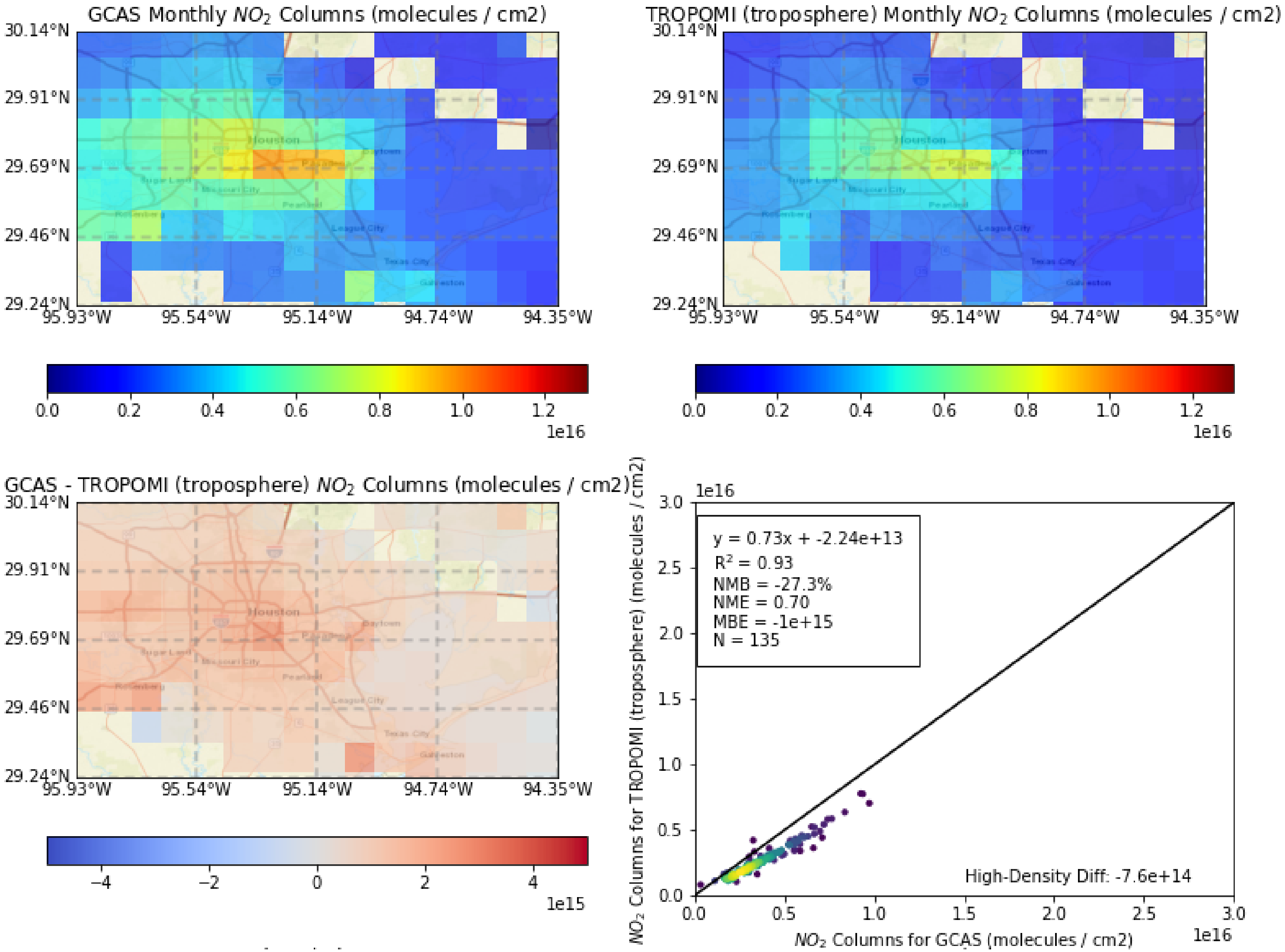


TROPOMI NO_2 v2.3.1 (CAMx AMF)





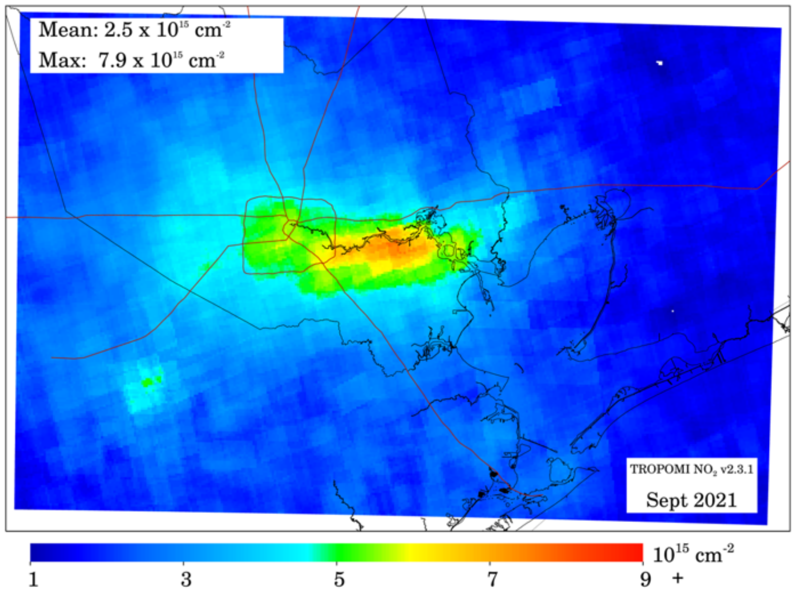


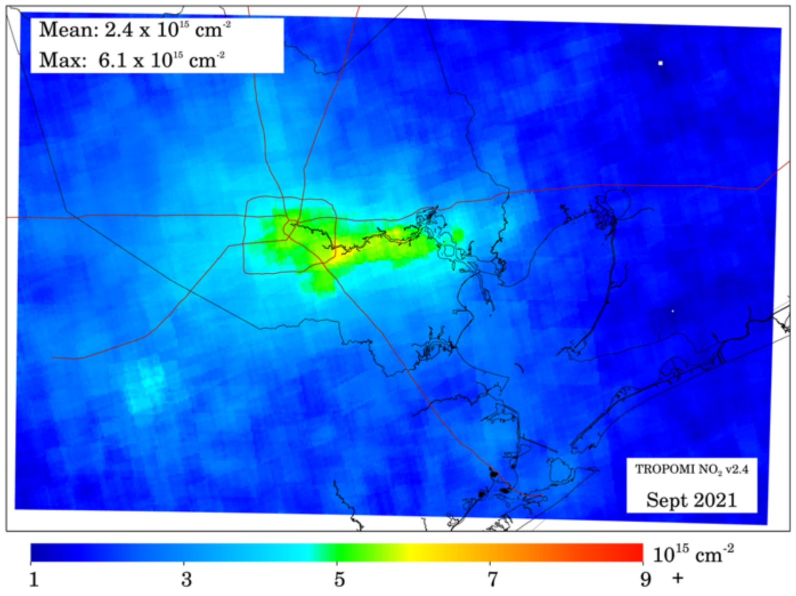


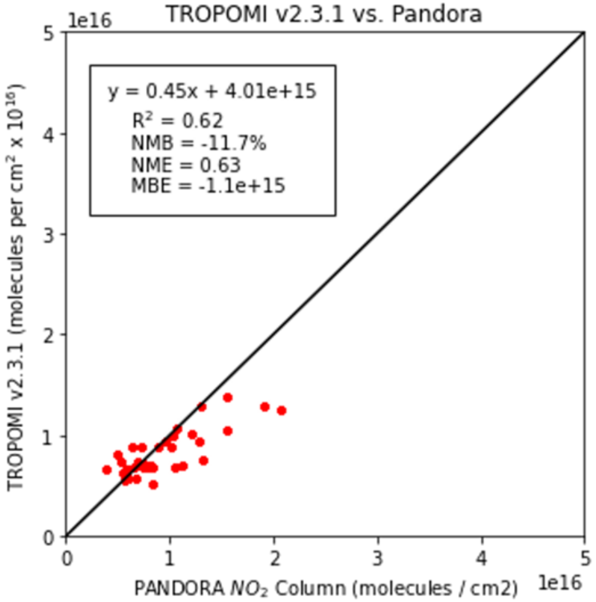
GCAS Monthly NO_2 Columns (molecules / cm2)
TROPOMI (troposphere) Monthly NO_2 Columns (molecules / cm2)
GCAS - TROPOMI (troposphere) NO_2 Columns (molecules / cm2)
30.14°N
29.91°N
29.69°N
29.46°N
29.24°N
95.93°W
95.54°W
95.14°W
94.74°W
94.35°W
Houston
1e16
1e15
y = 0.73x + -2.24e+13
R^2 = 0.93
NMB = -27.3%
NME = 0.70
MBE = -1e+15
N = 135
High-Density Diff: -7.6e+14
NO_2 Columns for TROPOMI (troposphere) (molecules / cm2)
NO_2 Columns for GCAS (molecules / cm2)

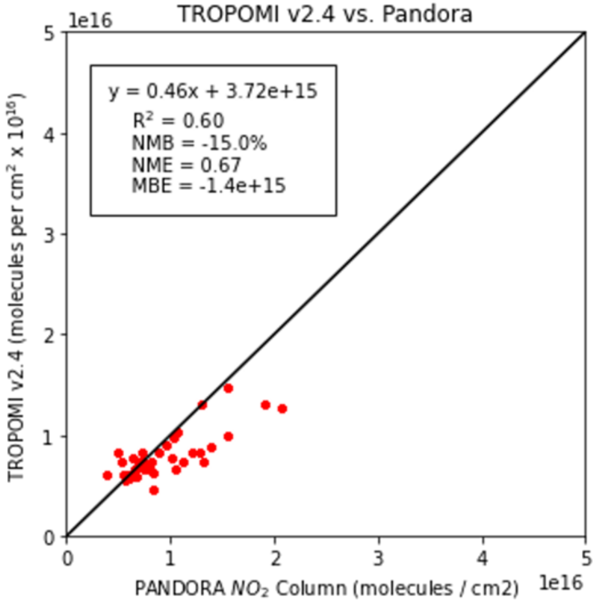
TROPOMI NO_2 v2.3.1

TROPOMI NO_2 v2.4



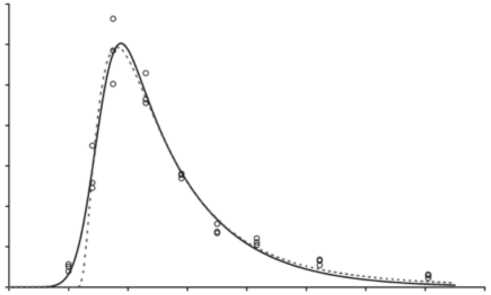






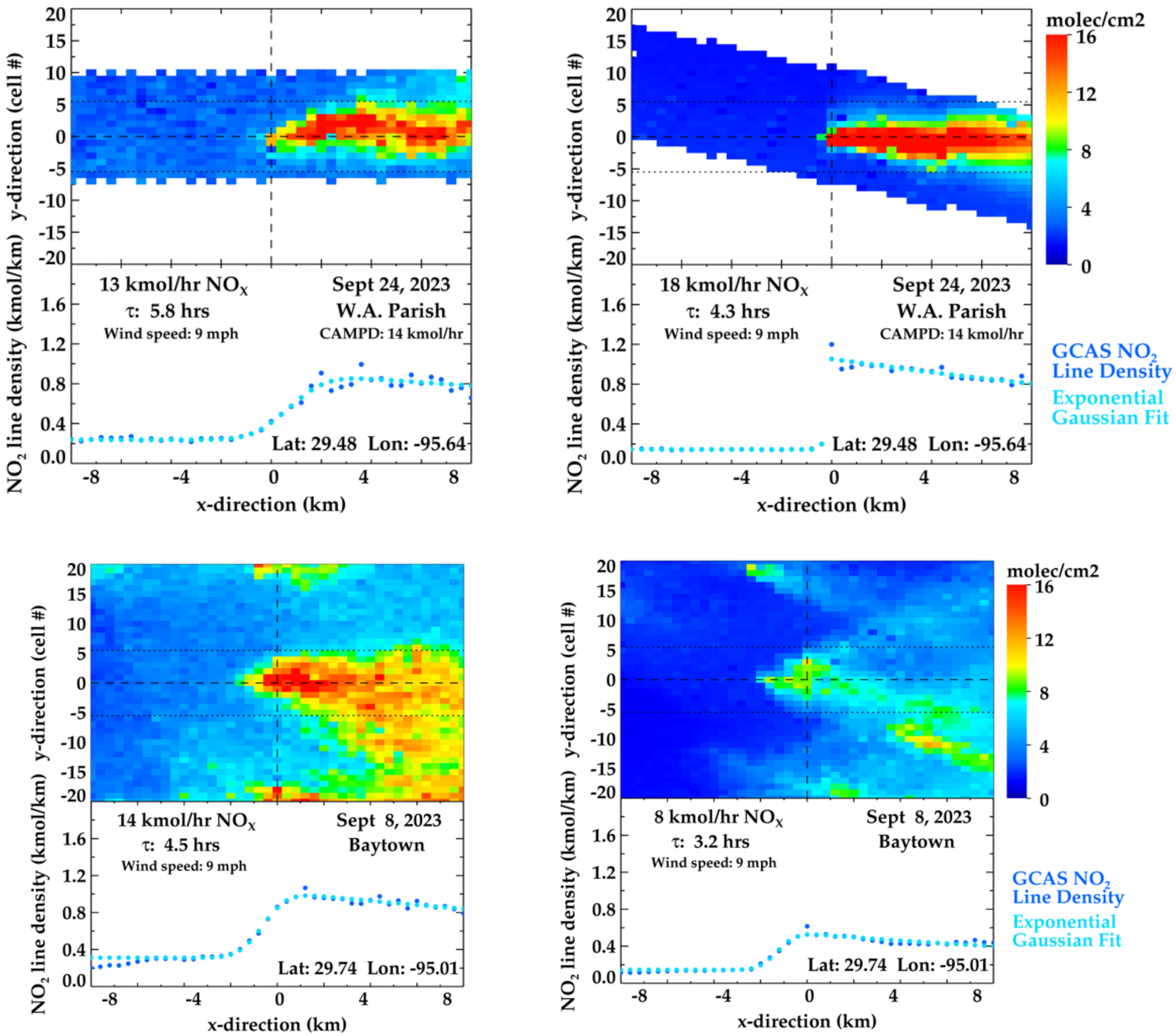
EMG fit

WA Parish PP
CAMPD: 14kmol/hr

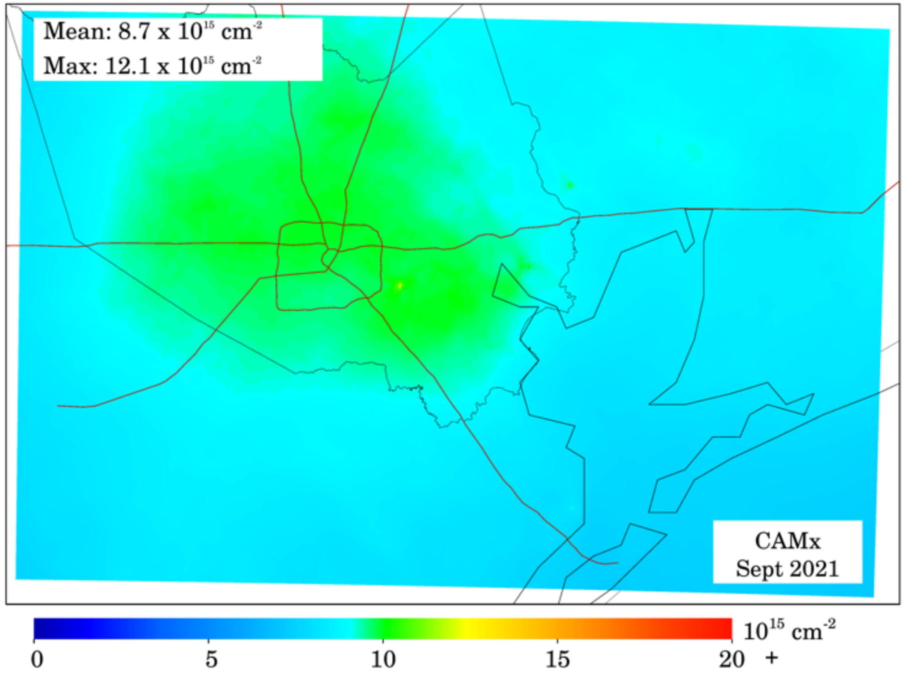


Baytown
CAMPD: N/A

GCAS **CAMx**



CAMx Column HCHO



TROPOMI Column HCHO