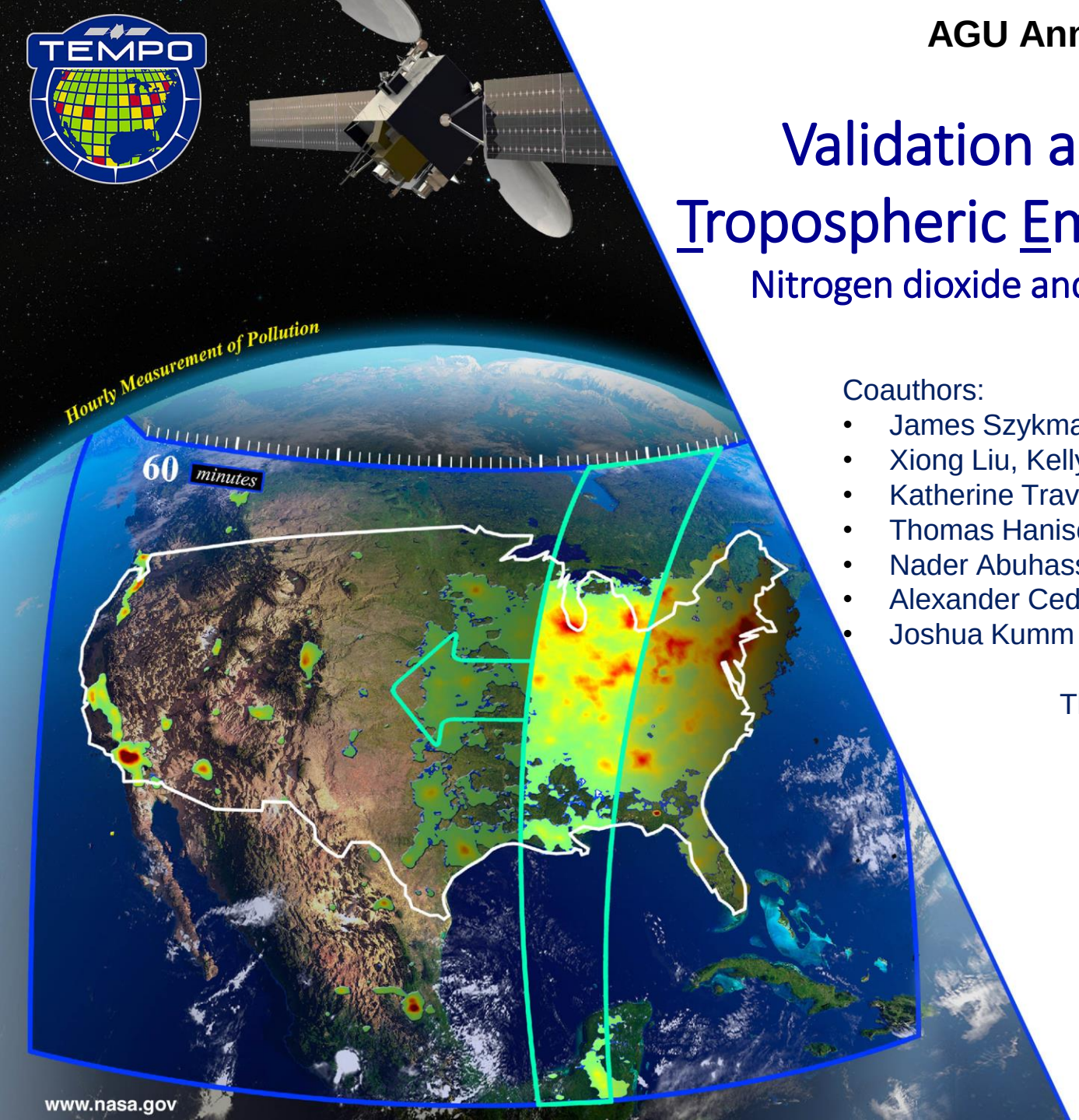


AGU Annual Meeting 9-13 December 2024

Validation and Early Applications of the Tropospheric Emission: Monitoring of POllution

Nitrogen dioxide and Formaldehyde using Pandora and TropOMI

Barron Henderson, US EPA

Coauthors:

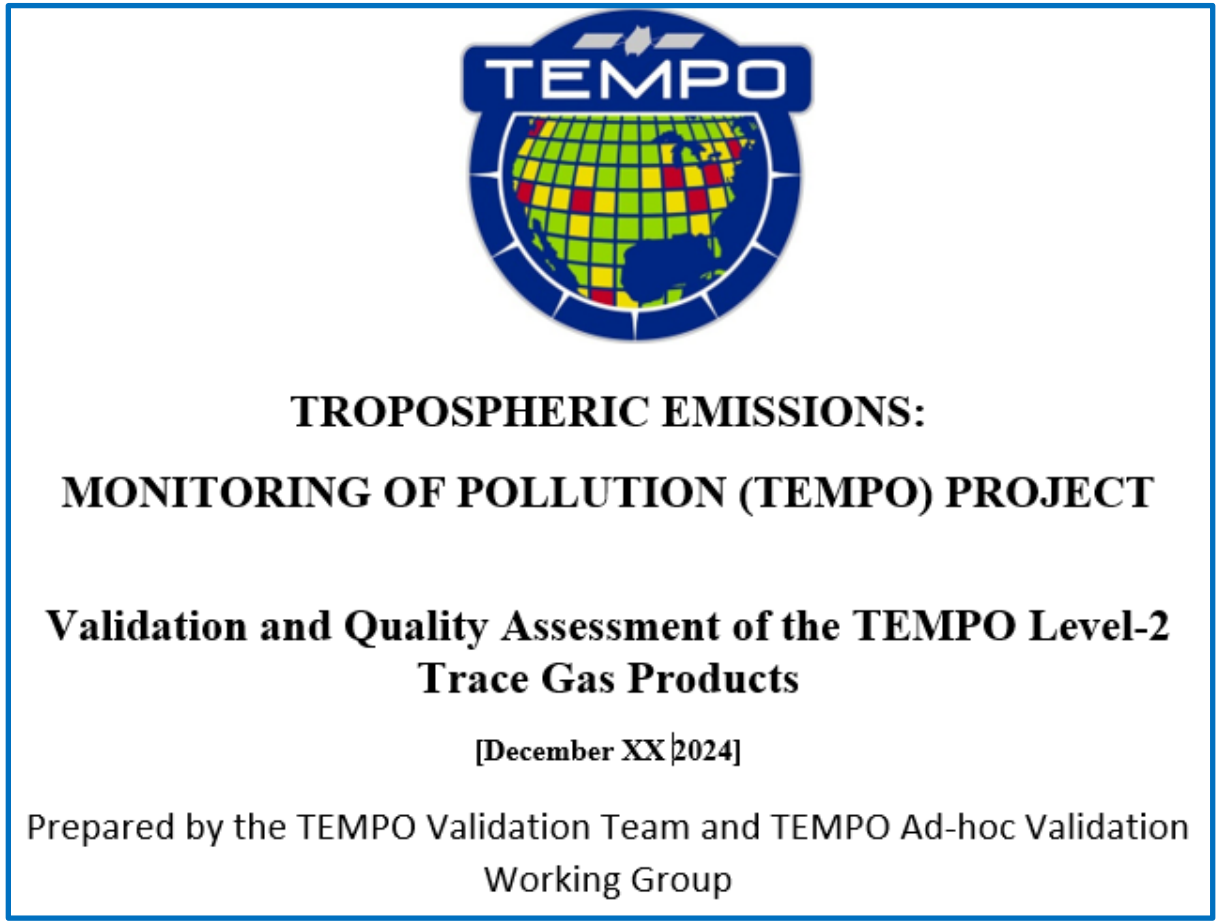
- James Szykman, Luke Valin, and Heather Simon, US EPA
- Xiong Liu, Kelly Chance, Gonzalo Gonzalez Abad, Caroline Nowlan, SAO TEAM
- Katherine Travis and Prajjwal Rawat, NASA LaRC
- Thomas Hanisco, NASA GSFC
- Nader Abuhassan, SciGlob
- Alexander Cede, LuftBlick
- Joshua Kumm and Zhen Qu, North Carolina State University

Thanks to the rest of the TEMPO Validation Team!

***Disclaimer**: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.*

NASA Smithsonian Ball UNITED STATES ENVIRONMENTAL PROTECTION AGENCY SSEC

Validation Efforts Help Advance TEMPO



TROPOSPHERIC EMISSIONS:

MONITORING OF POLLUTION (TEMPO) PROJECT

Validation and Quality Assessment of the TEMPO Level-2 Trace Gas Products

[December XX 2024]

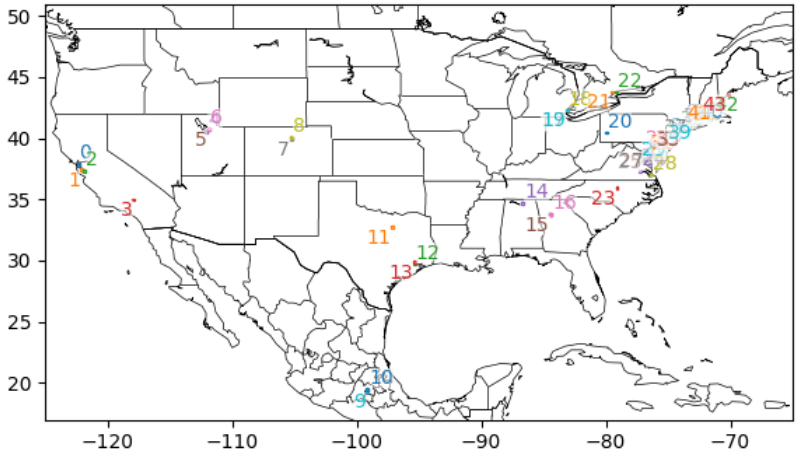
Prepared by the TEMPO Validation Team and TEMPO Ad-hoc Validation Working Group

Plan: available –https://tempo.si.edu under documents
Report: Draft ***under review***

- **Validation TEAM enhanced TEMPO mission**
  - 65+ contributors led by Jim Szykman (EPA) and Brad Pierce (UW-SEC) in collaboration with Science Team, NASA, NOAA, and SAO.
  - Expanded the Pandonia Global Network of Pandoras
  - Feedback about version 1 priori profile and unrealistic AMF spatial variation helped improve versions 2 and 3
  - Validation report submitted to NASA
  - including results shown today…
- ***EPA's Analysis System now V3***
  - V3 Nitrogen dioxide correlates well with Pandora and TropOMI.
  - V3 Formaldehyde correlates well with Pandora ...
- ***Example Applications of TEMPO with CMAQ***
  - Model evaluation and emissions inference.
  - Surface concentration experiments
  - *Very preliminary and expanding!*
- ***Applications presume validation!***

TEMPO Validation Methodologies

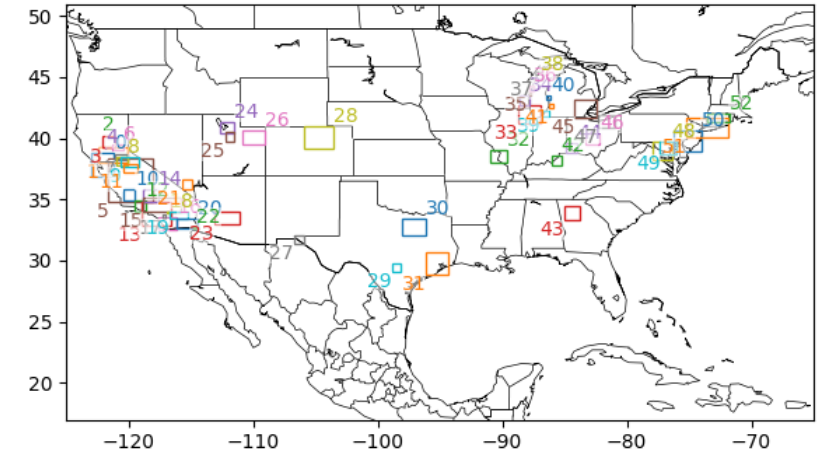
- **Correlative measurements : TropOMI and Pandora Spectrometers**
  - Pandora stations: best ground-based validation dataset available for total vertical columns.
  - TropOMI: state-of-the-art satellite retrievals at similar spatial resolution.
- **96 Analysis Regions: Pandonia Global Network and Ozone Nonattainment Areas.**



0: RichmondCA
1: MountainViewCA
2: SanJoseCA
3: EdwardsCA
4: SouthJordanUT
5: SLC-Hawthorne
6: SLC-UT
7: BoulderCO
8: BoulderCO-NCAR
9: MexicoCity-UNAM
10: MexicoCity-Vallejo
11: ArlingtonTX
12: HoustonTX
13: AldineTX
14: HuntsvilleAL
15: AtlantaGA
16: Atl-S.DeKalb
17: DearbornMI
18: SWDetroitMI
19: Windsor-West
20: PittsburghPA
21: Downsview
22: Toronto-Scarborough
23: ChapelHillNC
24: CharlesCityVA
25: WashingtonDC
26: BeltsvilleMD
27: GreenbeltMD
28: HamptonVA-HU
29: PhiladelphiaPA
30: BristolPA
31: NewBrunswickNJ
32: BayonneNJ
33: ManhattanNY-CCNY
34: BronxNY
35: QueensNY
36: WestportCT
37: CornwallCT
38: OldFieldNY
39: NewHavenCT
40: MadisonCT
41: LondonderryNH
42: EastProvidenceRI
43: CapeElizabethME

- 44 **Pandora** stations
- Most stations in the east

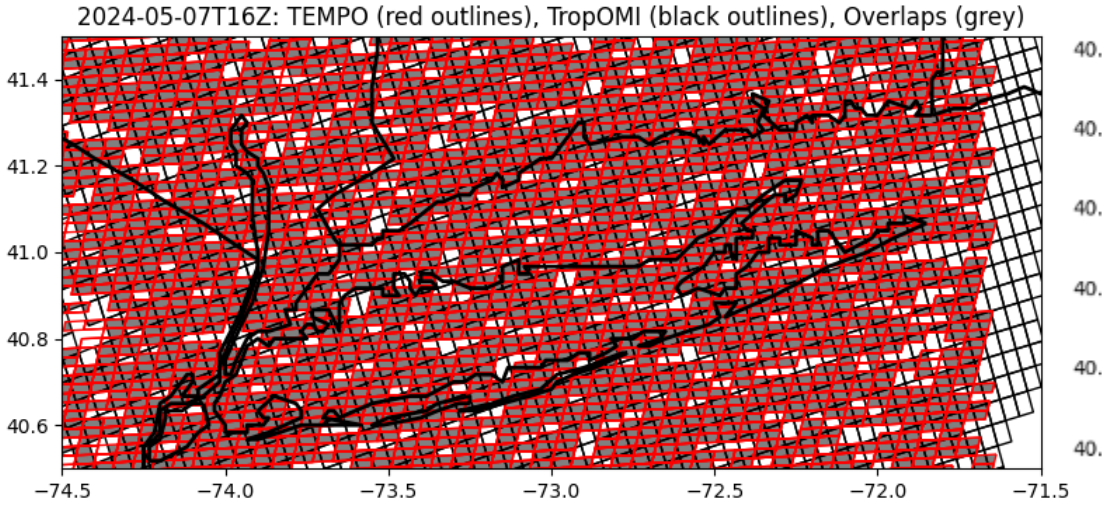
- 52 **Nonattainment Areas**
- Better spatial coverage
- Of special interest for emissions control

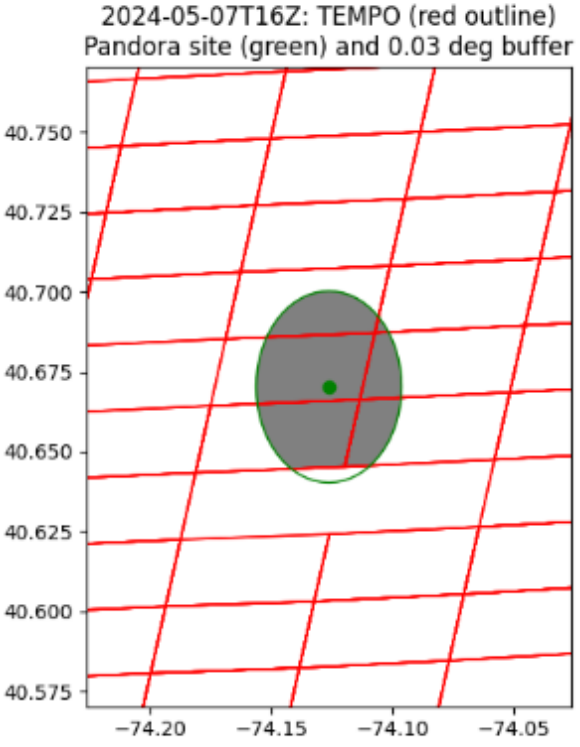


0: S.Francisco
1: Sacramento
2: Tuscan_Buttes
3: Chico
4: Sutter_Buttes
5: S.Joaquin
6: Nevada_Co
7: Amador_Co
8: Calaveras_Co
9: Tuolumne_Co
10: S.Luis_Obispo
11: Mariposa_Co
12: Ventura_Co
13: LA-S_Coast
14: East_Kern
15: LA-Desert
16: S.Diego
17: Pechanga
18: Morongo
19: Coachella_Val
20: Imperial_Co
21: Las_Vegas
22: Yuma
23: Phoenix
24: Salt_Lake
25: Provo
26: Uinta_Basin
27: El_Paso
28: Denver
29: S.Antonio
30: Dallas
31: Houston
32: St_Louis
33: Chicago
34: Milwaukee
35: Sheboygan
36: Manitowoc_Co
37: Door_Co_Rev
38: Door_Co
39: Benton_Harbor
40: Muskegon
41: Allegan_Co
42: Louisville
43: Atlanta
44: Cincinnati
45: Detroit
46: Columbus
47: Cleveland
48: Washington
49: Baltimore
50: Philadelphia
51: New_York
52: Connecticut

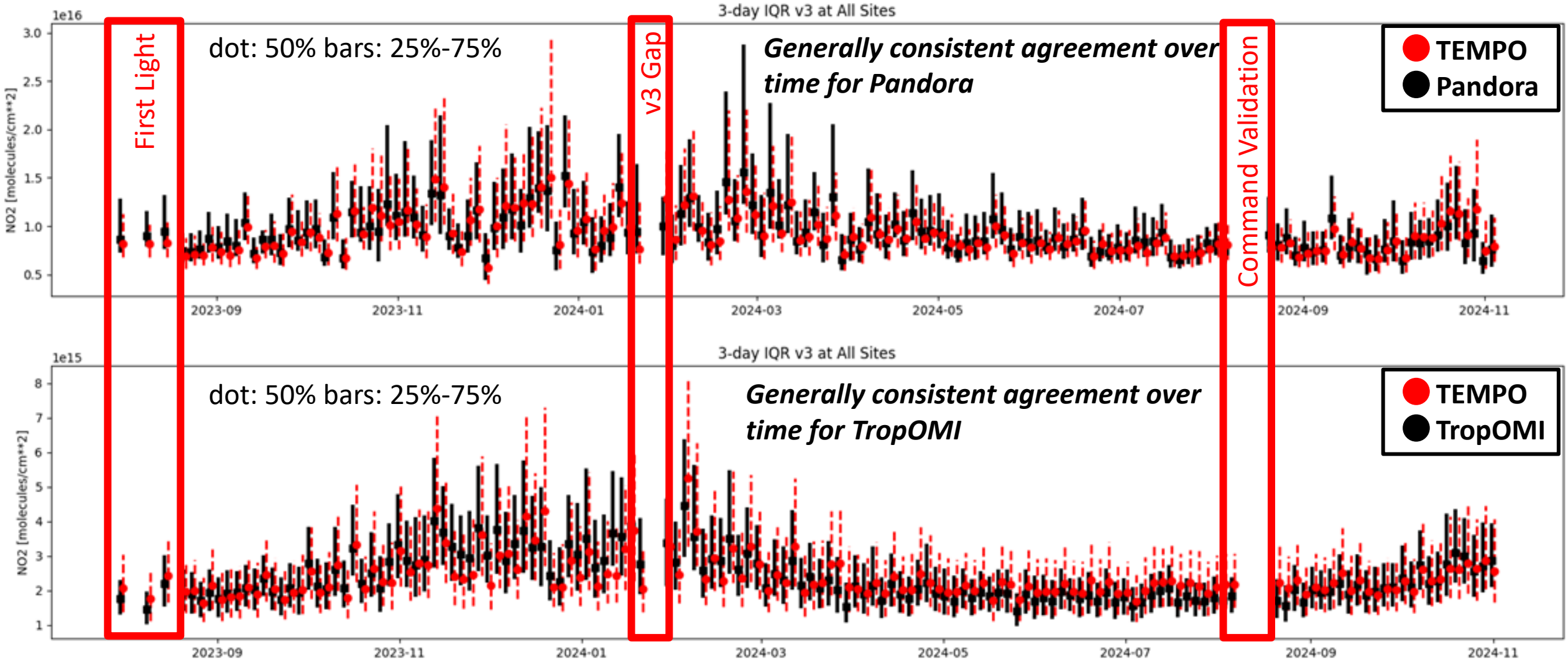
TEMPO Validation Methodologies

- **Get level 2 data for TEMPO, TropOMI, and Pandora**
  - Python bindings for EPA's Remote Sensing Information Gateway (pyrsig)
  - Trainings available – see QR code
- **Select time intersections**
  - TropOMI: same hour (e.g., 19:00:00Z to 19:59:59Z)
  - Pandora: overpass within 15min of observation
- **Select spatial intersections**
  - TropOMI: pixels overlap
  - Pandora: overlap a buffer
- **Pool intersections for statistical analyses**
  - Pixels near Pandora locations
  - Pixels in Nonattainment areas

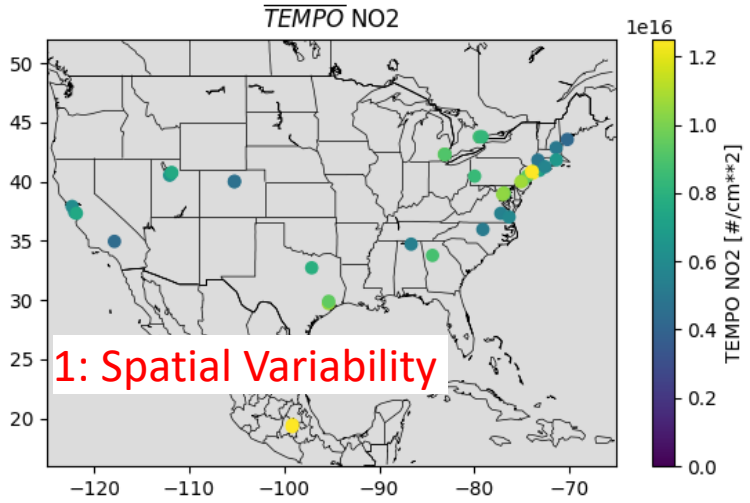


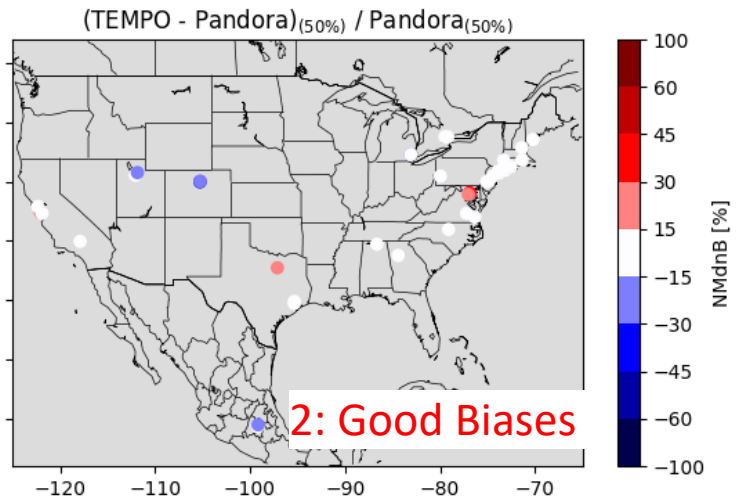


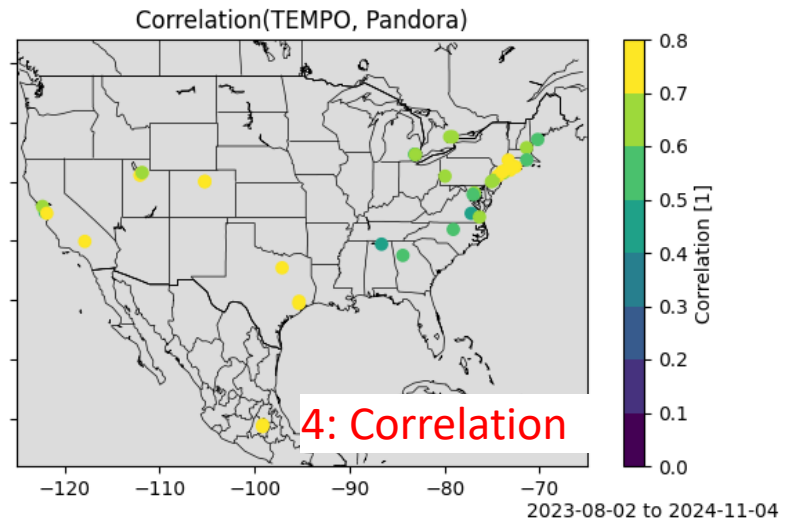
NO2 Data Record Overview
All Intersections Aug 2023 to Oct 2024

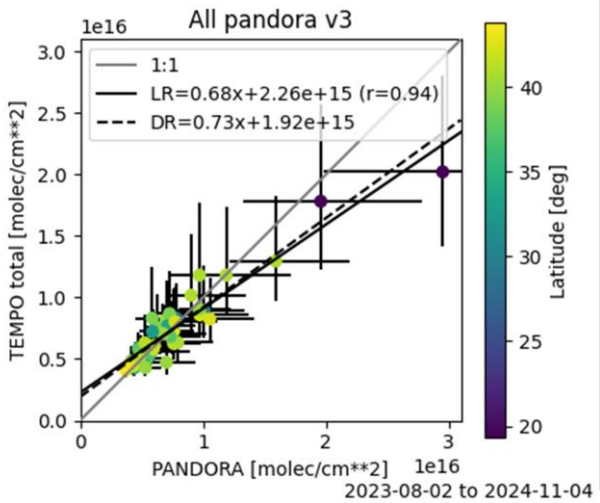


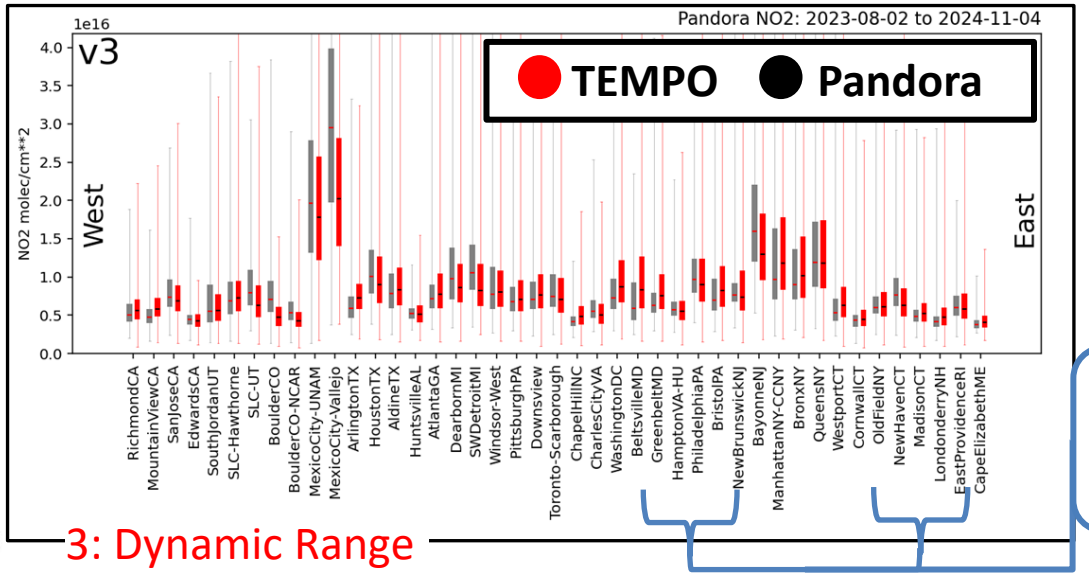
TEMPO L2 NO_2 agrees well with Pandora







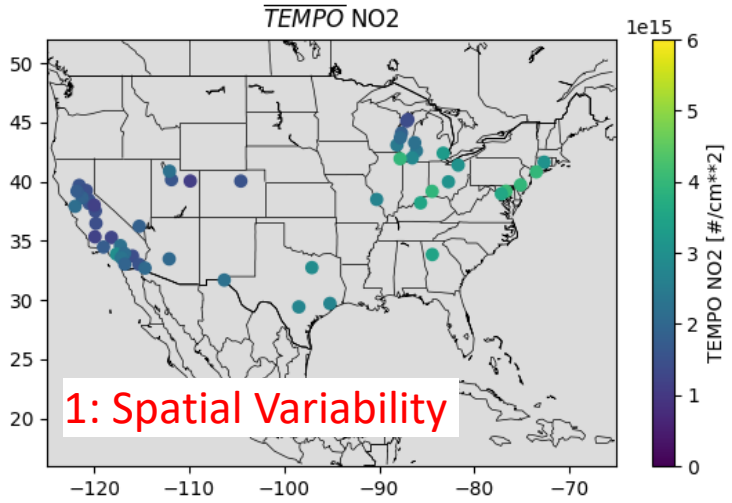


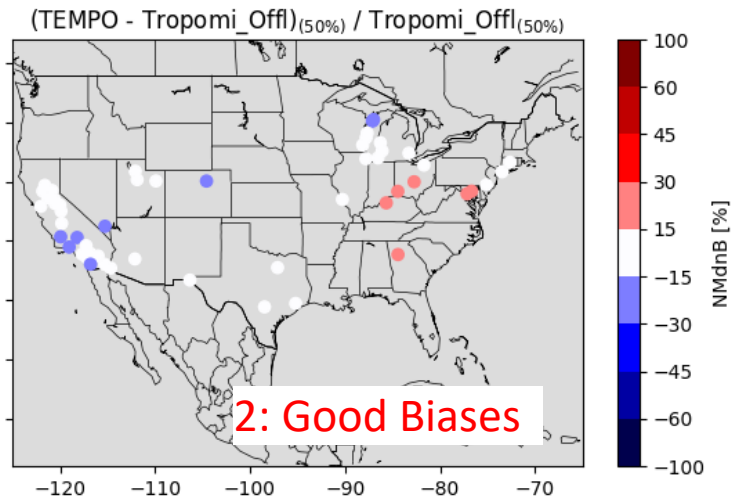


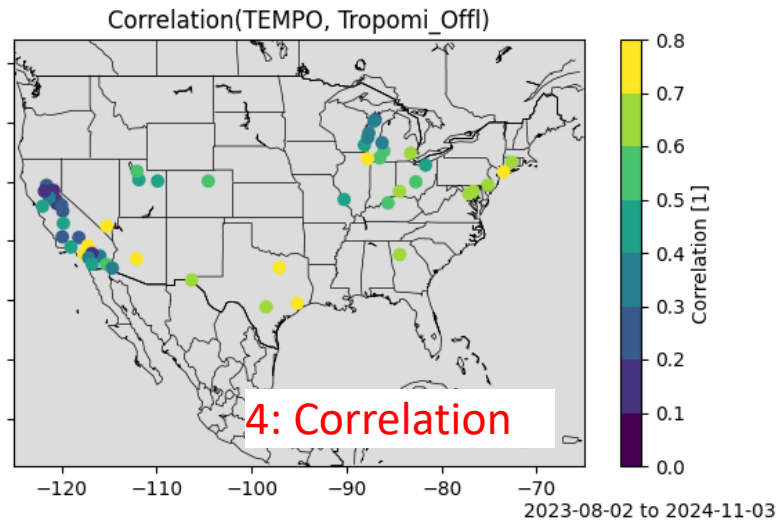
Compared to Pandora direct sun measurements, TEMPO:

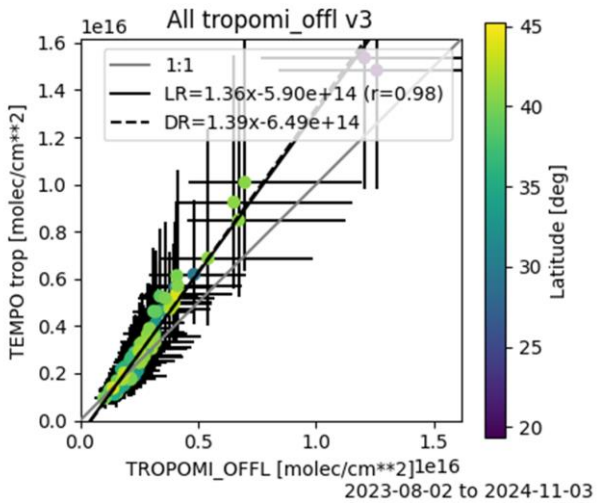
1. Reproduces spatial variability
2. Low fractional biases by locations.
3. Reproduces dynamic range by site
4. Correlates well at most sites.
5. Even reproduces relatively small intra-regional urban/rural gradients quite well.

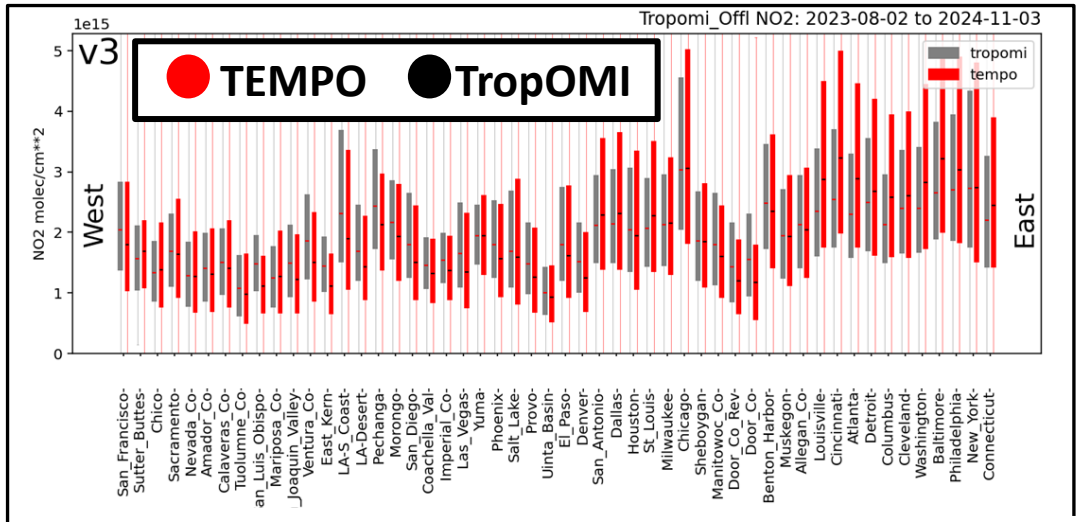
TEMPO L2 NO_2 agrees well with TropOMI











3: Dynamic Range —O3: Ozone Nonattainment Areas

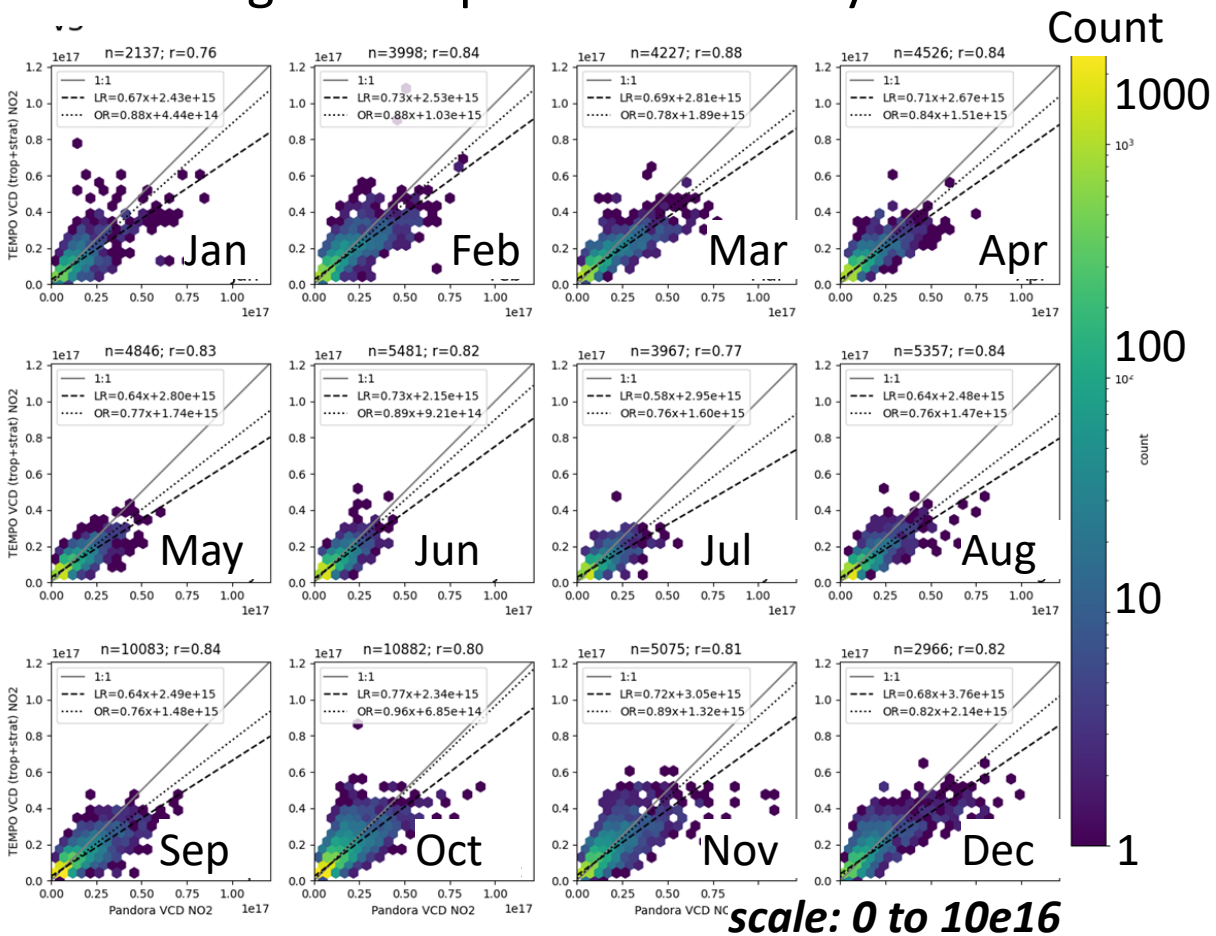
- TropOMI correlation is useful because we don't have Pandora everywhere.
- Here we explore comparisons at Ozone Nonattainment Areas
- Similar story to Pandora/TEMPO, captures spatial variability, dynamic range with a mix of site-specific correlations.
- Higher slope than Pandora, but this is tropospheric column.

Seasonal and Diurnal Performance is Consistent

TEMPO L2 vs Pandora Total NO2

Consistent monthly performance

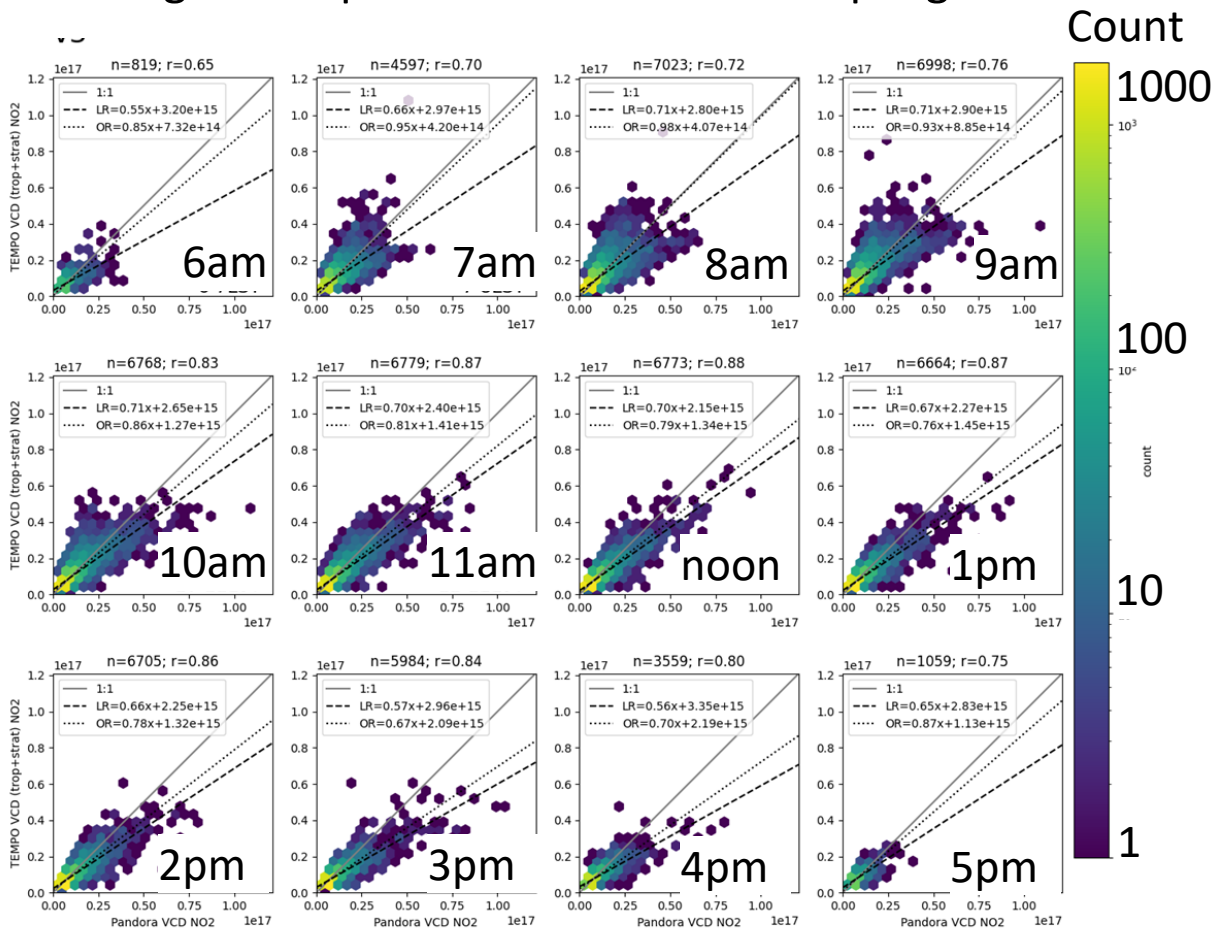
- Dynamic range varies by month as expected
- Orthogonal slopes consistent by month



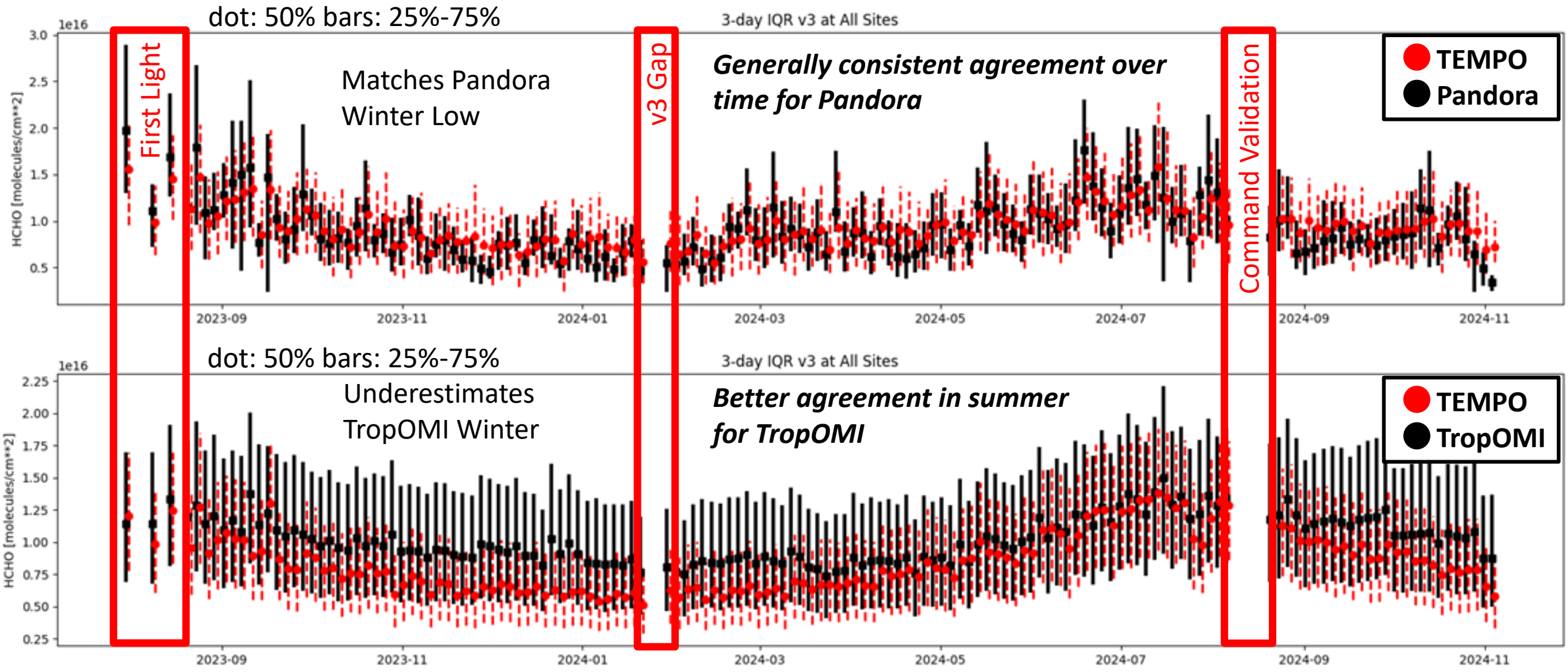
scale: 0 to 10e16

Consistent diurnal performance

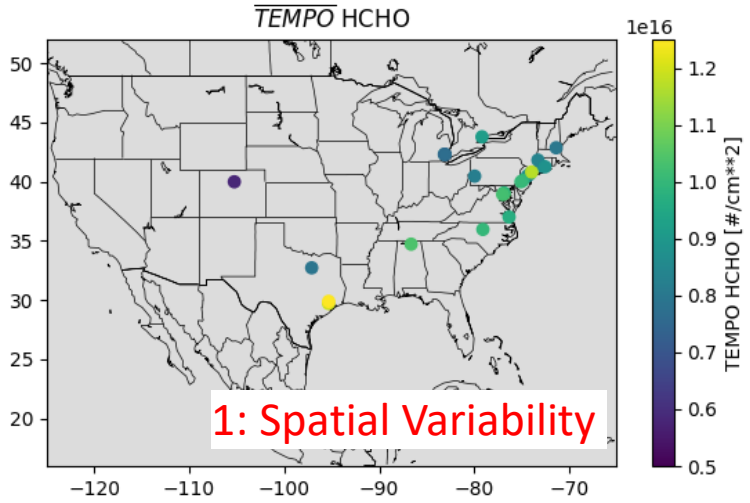
- Dynamic range varies by time of day as expected
- Orthogonal important due airmass sampling.

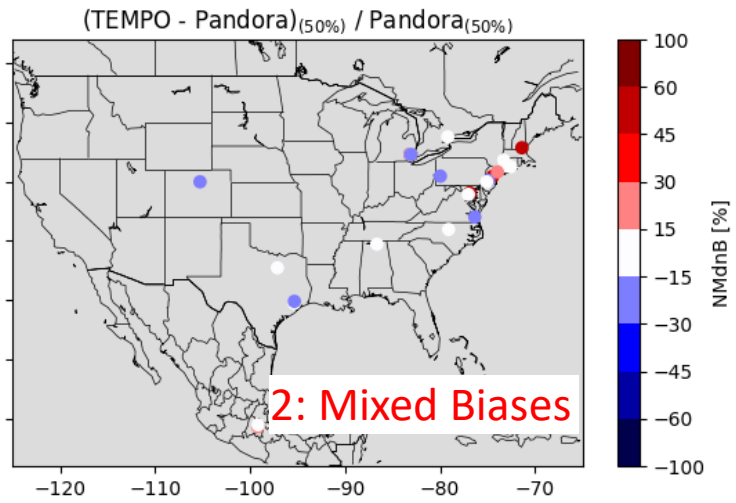


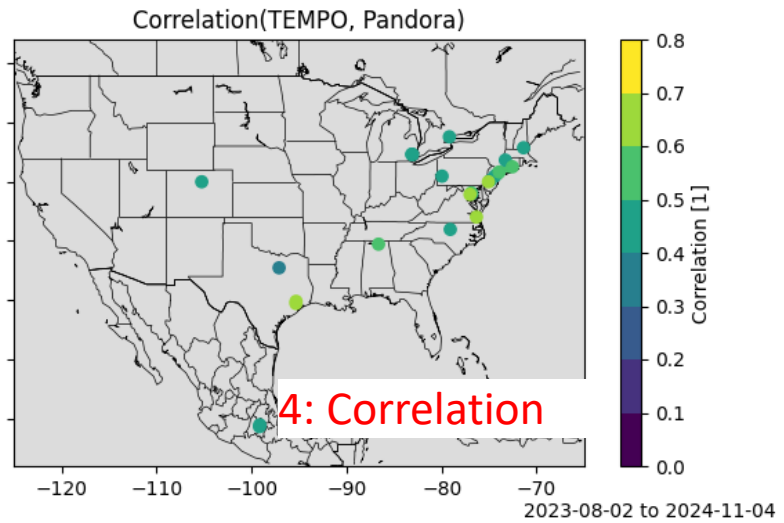
HCHO Data Record Overview
All Intersections Aug 2023 to Oct 2024

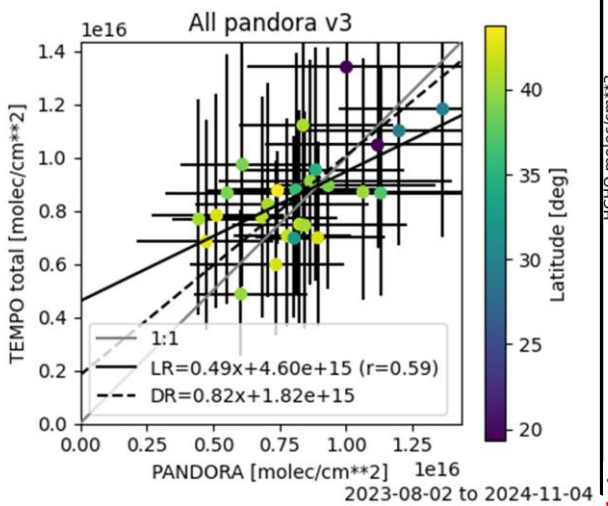


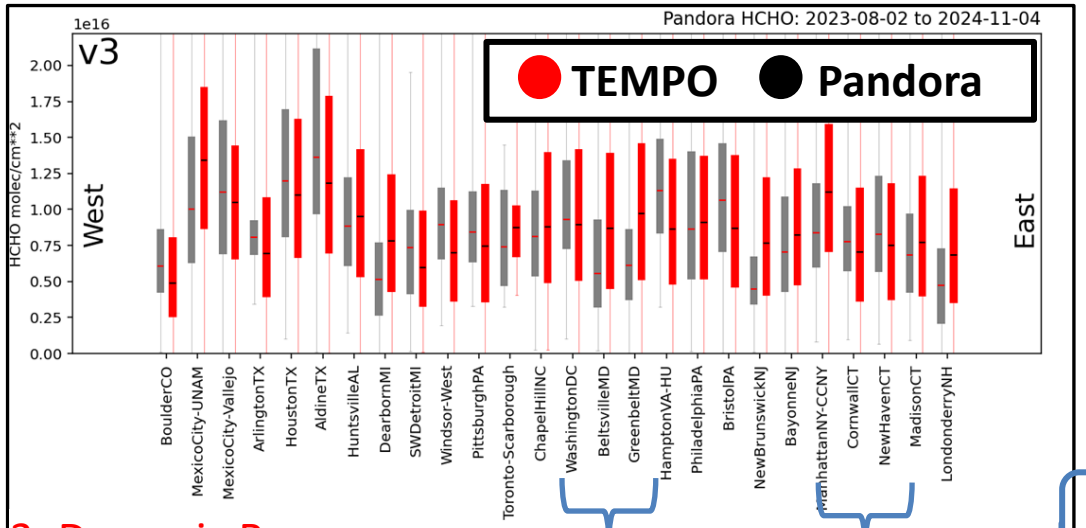
TEMPO L2 HCHO agrees with Pandora











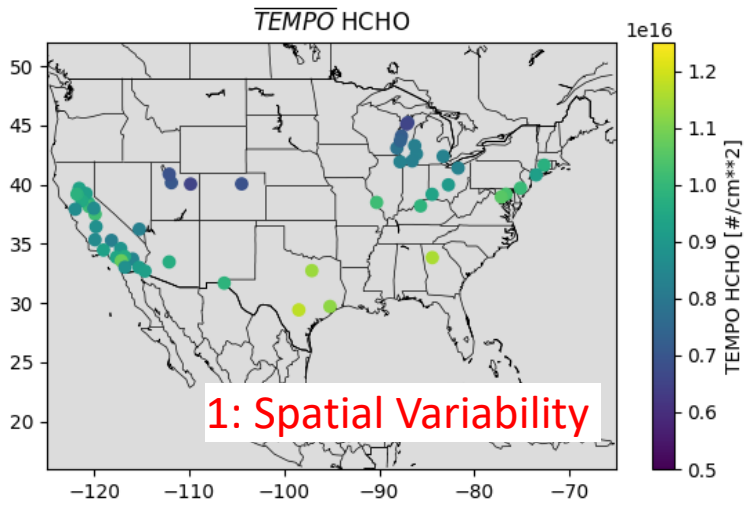
Using direct sun with pixel averaging

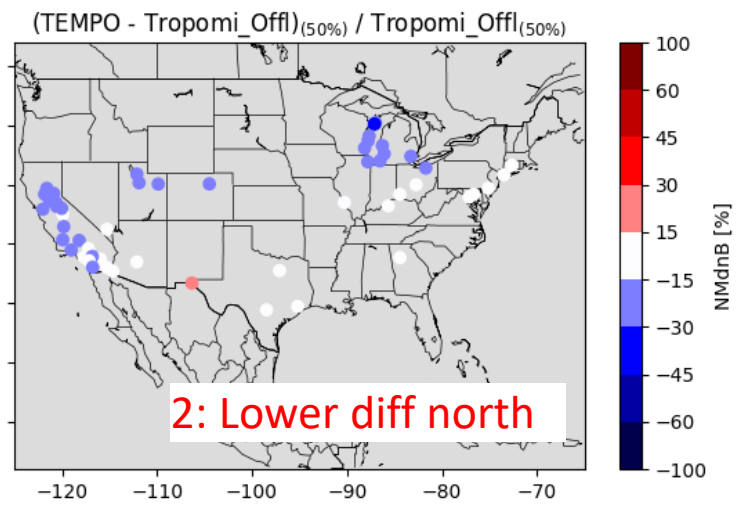
- Site selection: direct sun vs sky scan
- *See Prajjwal Rawat for more details*

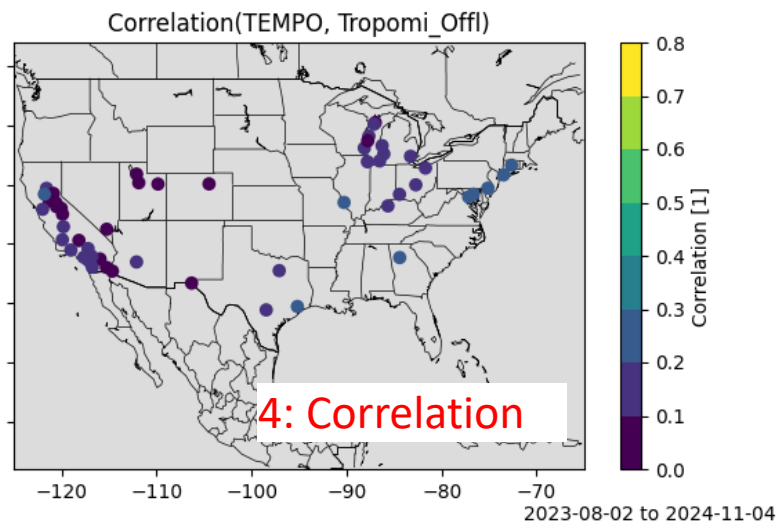
Compared to Pandora, TEMPO:

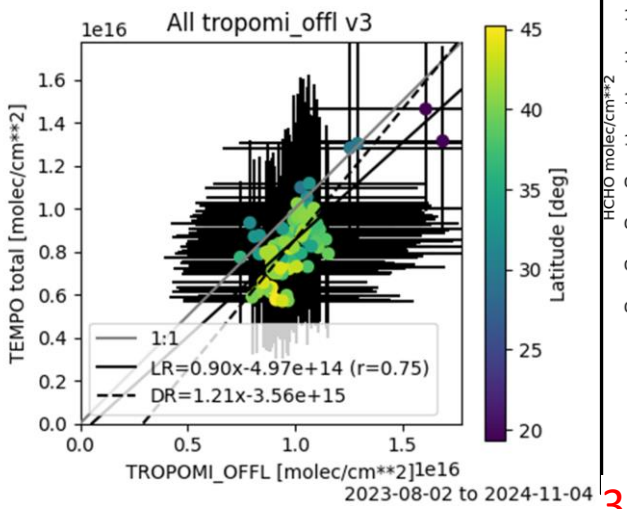
1. Correlates at the site-level
2. Has reasonable bias with some individual sites needing investigation.
3. Captures regional-specific dynamic range.
4. Site-specific time correlation.
5. Intra-regional site-level gradients are challenging, perhaps due to pixel averaging

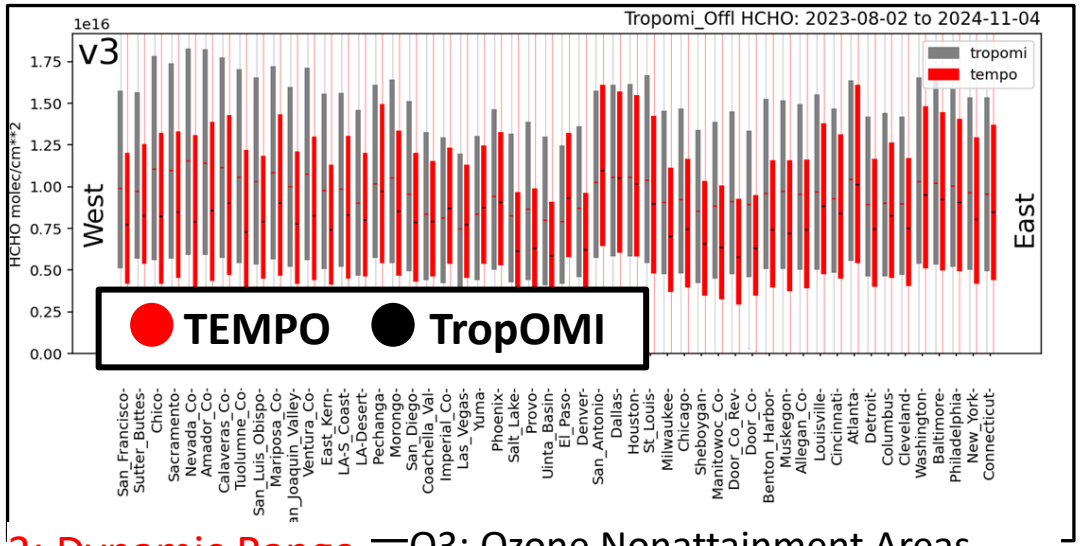
TEMPO L2 HCHO agrees with TropOMI











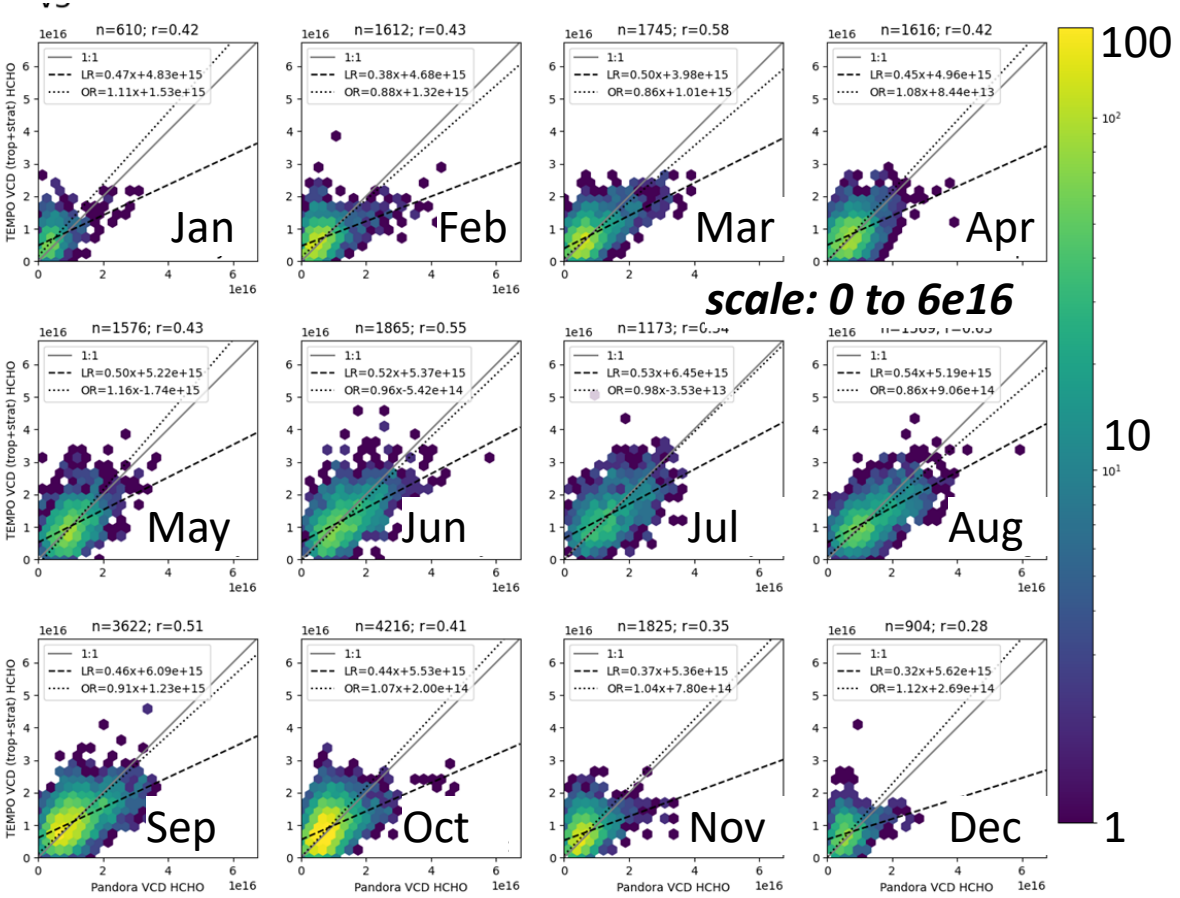
- TropOMI correlation is useful because we don't have Pandora everywhere.
- Here we explore comparisons at Ozone Nonattainment Areas
- Unlike NO2, the diurnal cycle of HCHO is not strong many places which implicitly makes temporal correlation more challenging.

Seasonal and Diurnal Performance is Consistent

TEMPO L2 vs Pandora Total HCHO

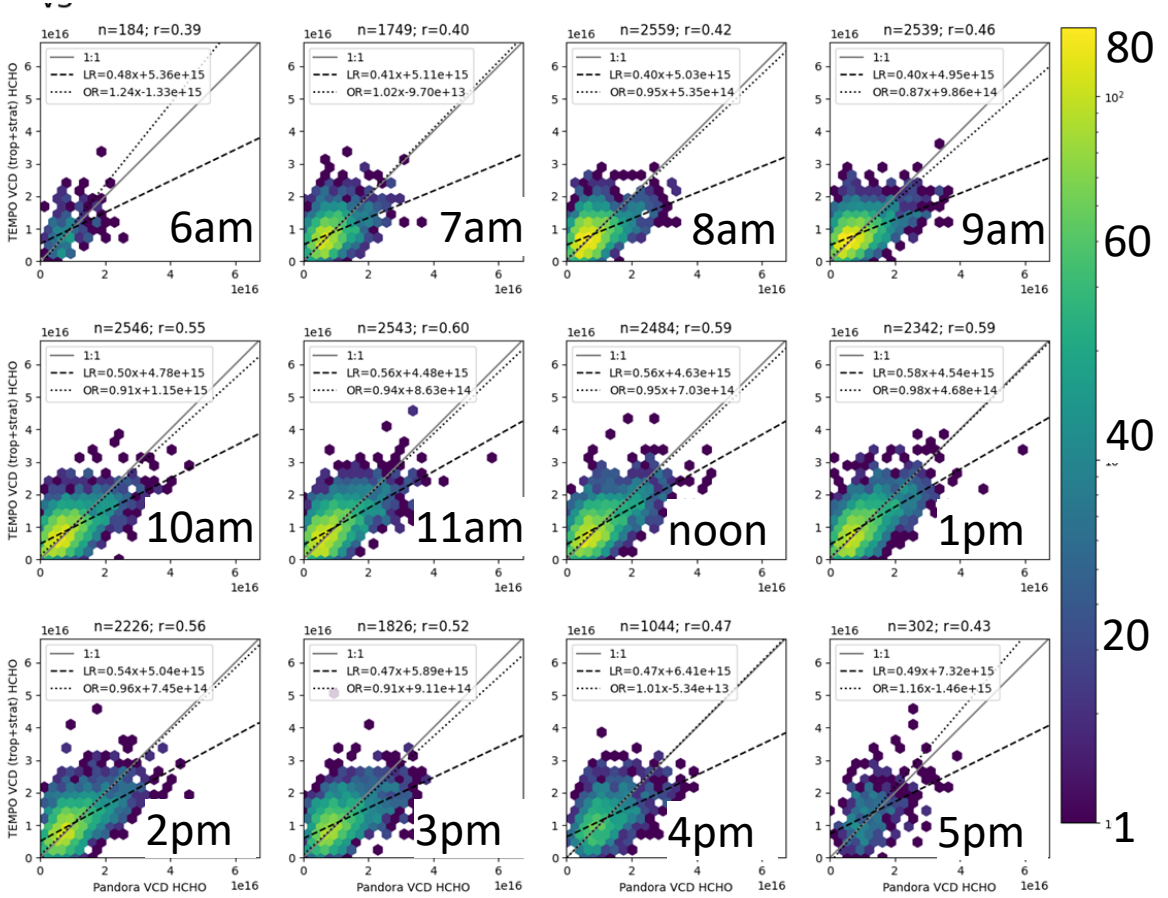
Consistent monthly performance

- Dynamic range varies by month as expected
- Orthogonal slopes consistent



Consistent diurnal performance

- Dynamic varies less by time of day
- Orthogonal important due airmass sampling.

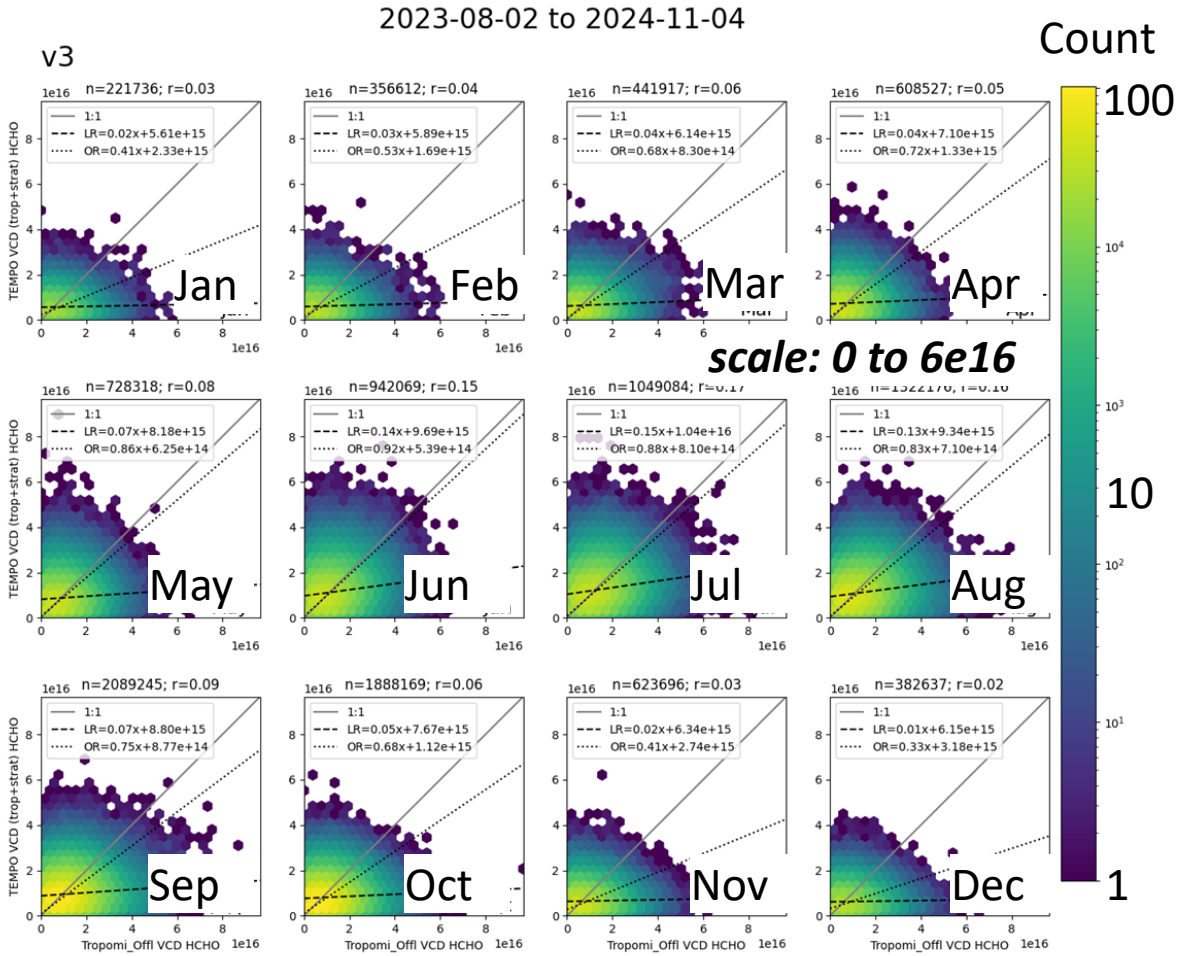


Seasonal and Diurnal Performance is Consistent

TEMPO L2 vs TropOMI Total HCHO

Better Agreement in Summer

- Dynamic range varies by month as expected
- Larger seasonal changes in TEMPO than TropOMI.
- Orthogonal slopes lowest in winter
  - Steadily increasing from January to May
  - Decreasing after August
- By comparison, Pandora slopes were quite consistent.
- Suggest looking into potential TropOMI high-bias in Winter/Spring

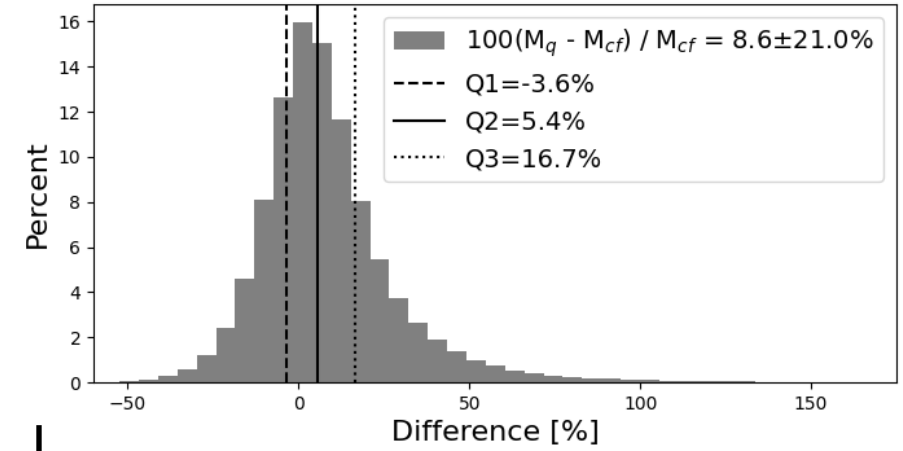


Early Applications

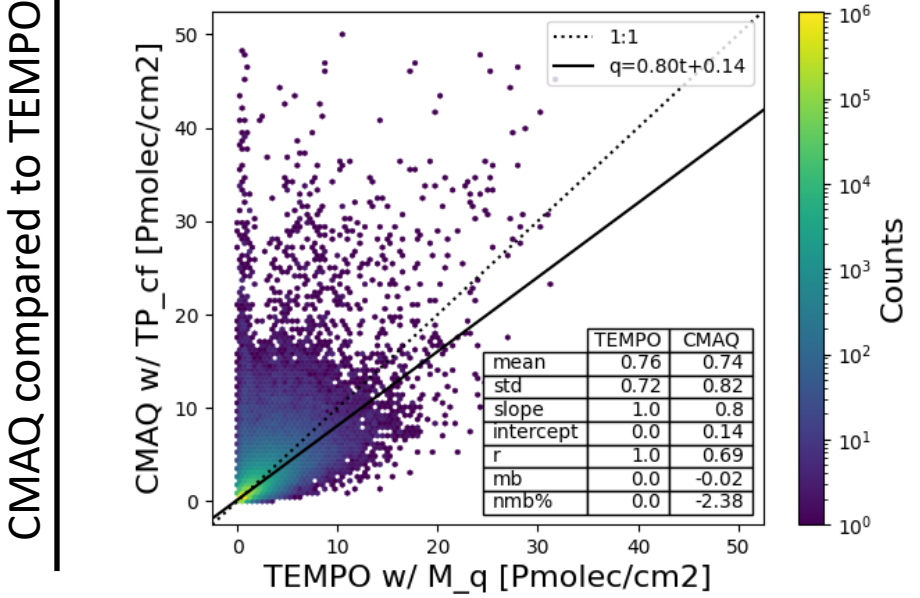
TEMPO L2 vs Preliminary CMAQ Application

- Focusing on NO2 Applications
  - Model performance evaluation (are columns similar?)
  - Dynamic evaluation (do columns respond to emissions similarly? Using weekend vs weekday
- Case study of convenience Sept 2023
  - Expediated Modeling of Burn Events Results (EMBER)*
    - 2018 anthropogenic emissions
    - 2023 preliminary fire inventory
  - *Longer analysis would be ideal*
- Consistent Atmospheric Shape Factor
  - CMAQ TropVCD: $\sum \Omega_{z,q}$
  - TEMPO TropVCD: TropSCD / M_q
  - Air Mass Factor: $M_q = \sum w_z \Omega_z \alpha(T_z) / \sum \Omega_{z,q}$
  - where z : $P_{z,mid} > P_{tropopause,cf}$

Air Mass Factor differences from TEMPO prior



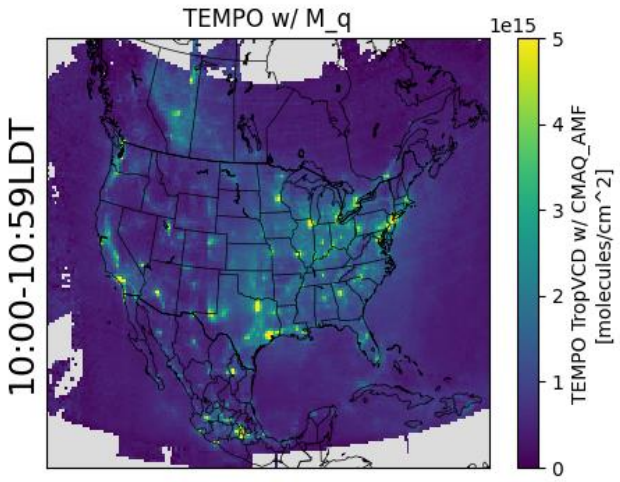
CMAQ compared to TEMPO

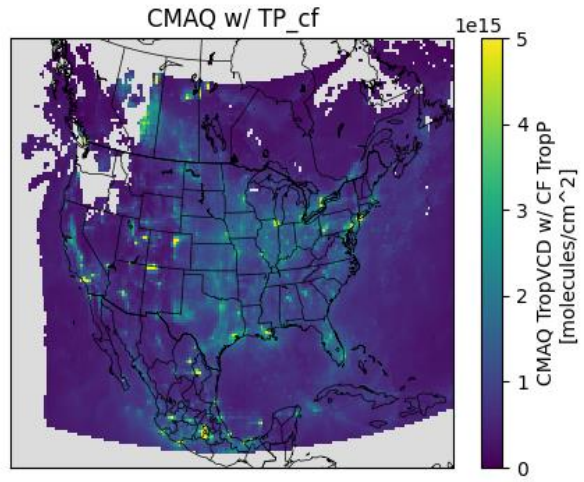


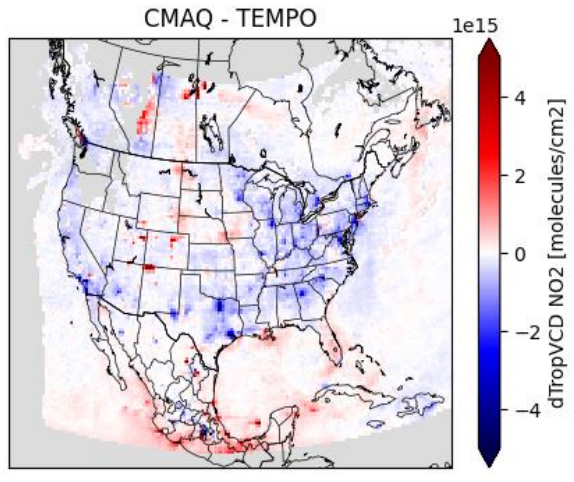
* Simon et al. (10.1016/j.dib.2024.111208) Data in Brief

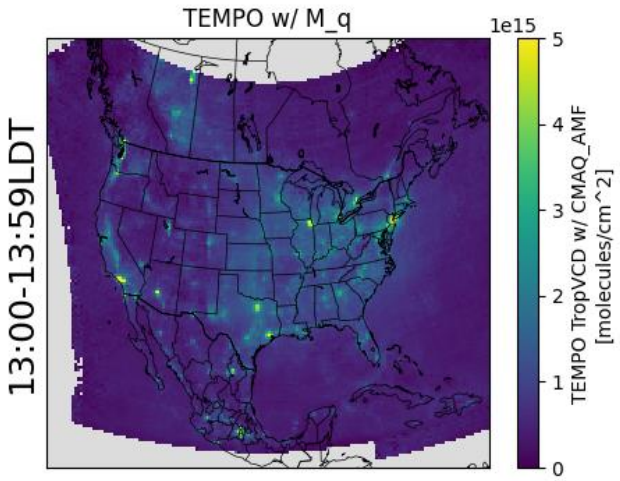
Model Performance Evaluation

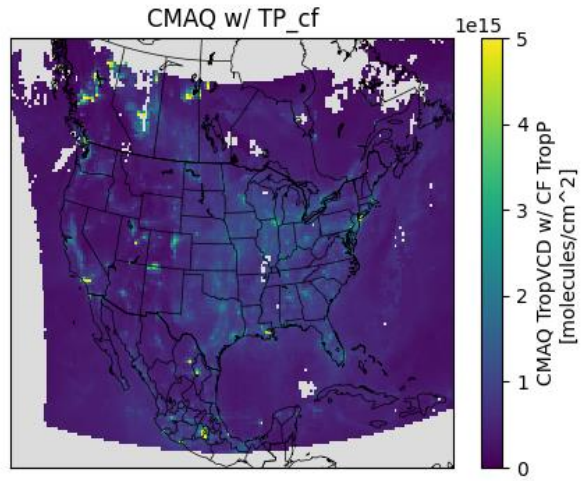
TEMPO L2 vs Preliminary CMAQ Application

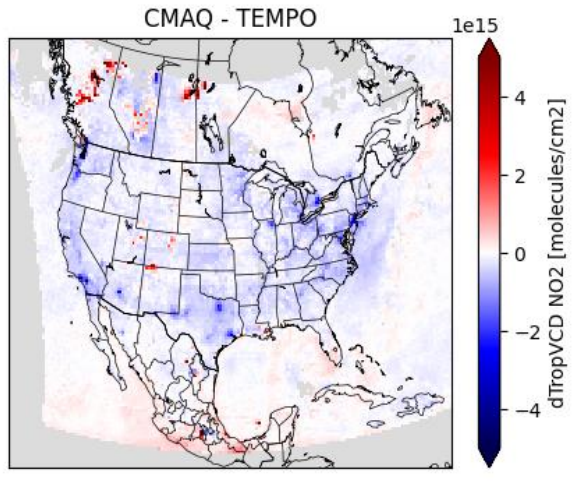












TEMPO TropVCD

CMAQ TropVCD

CMAQ – TEMPO

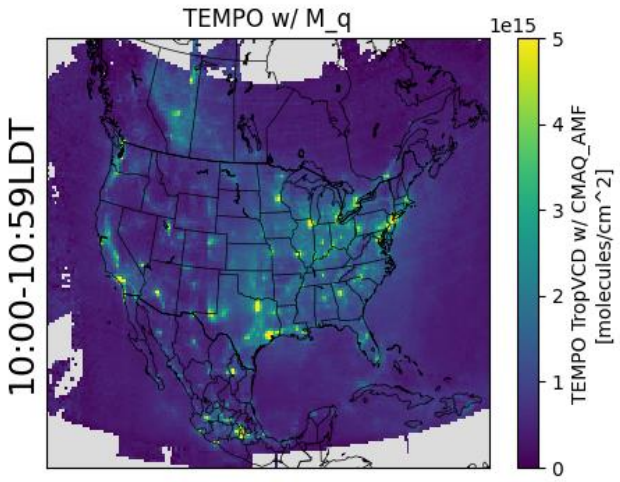
Sept 2023 average

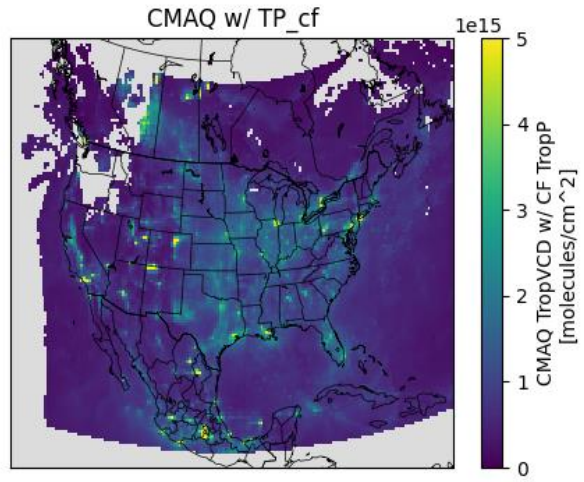
- CMAQ has low biases in many major cities
- TEMPO and CMAQ have larger tropospheric columns in the morning hours (10-11LDT) than at polar overpass.
- Morning differences are larger in absolute scale.

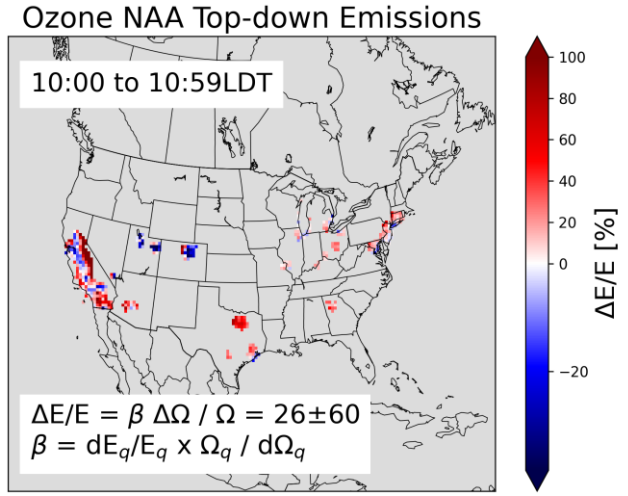
Consistent w/ Nash et al. 2024 (10.5194/egusphere-2024-554), corrects low ozone bias that is largest in the west.

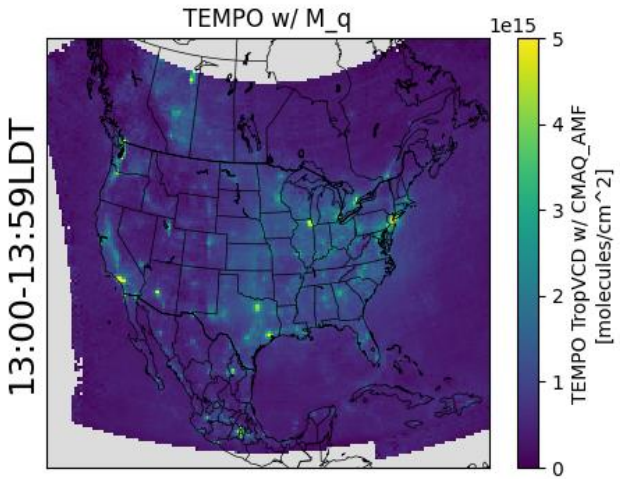
Model Performance Evaluation

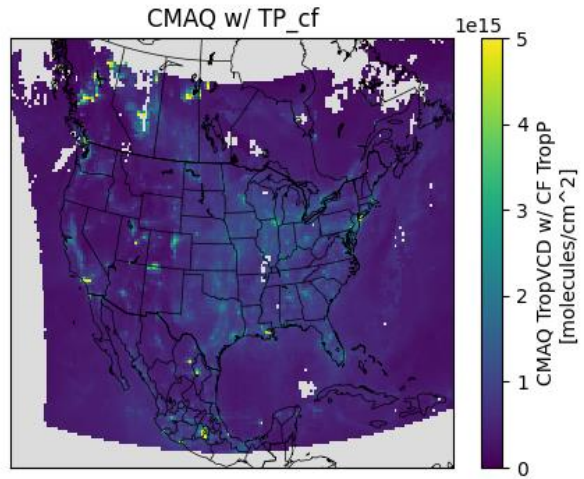
TEMPO L2 vs Preliminary CMAQ Application

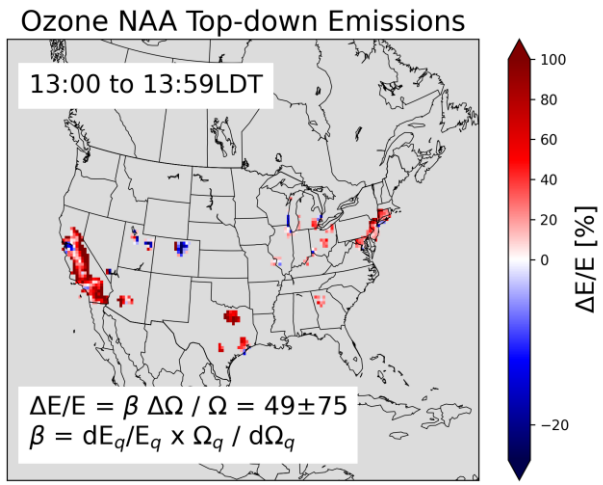












TEMPO TropVCD

CMAQ TropVCD

CMAQ – TEMPO

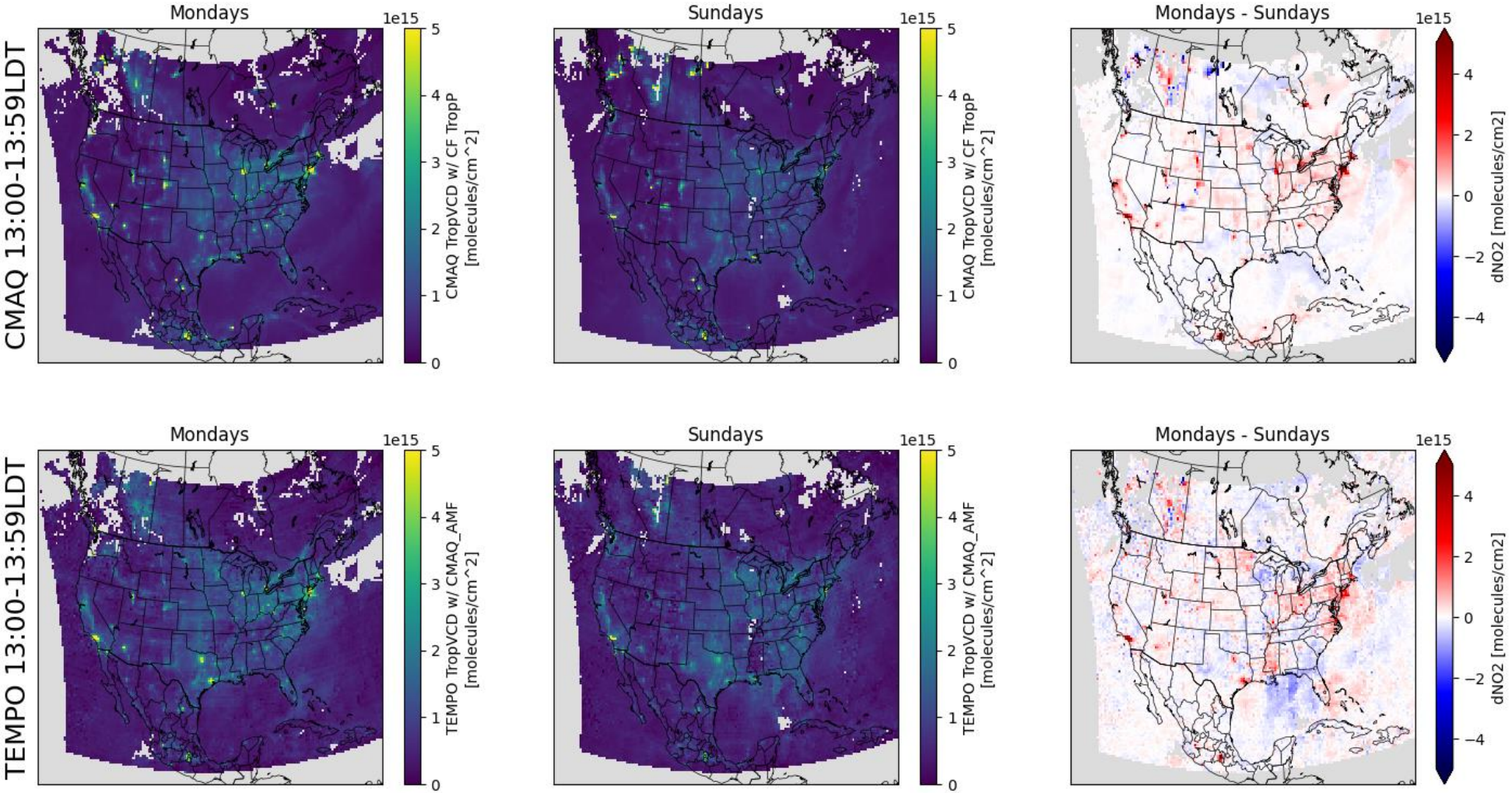
Sept 2023 average

- CMAQ has low biases in many major cities
- TEMPO and CMAQ have larger tropospheric columns in the morning hours (10-11LDT) than at polar overpass.
- Morning differences are larger in absolute scale.
- Mass balance inversion

Consistent w/ Nash et al. 2024 (10.5194/egusphere-2024-554), corrects low ozone bias that is largest in the west.

Dynamic Evaluation

TEMPO L2 vs Preliminary CMAQ Application



Monday Magnitude

Sunday Magnitude

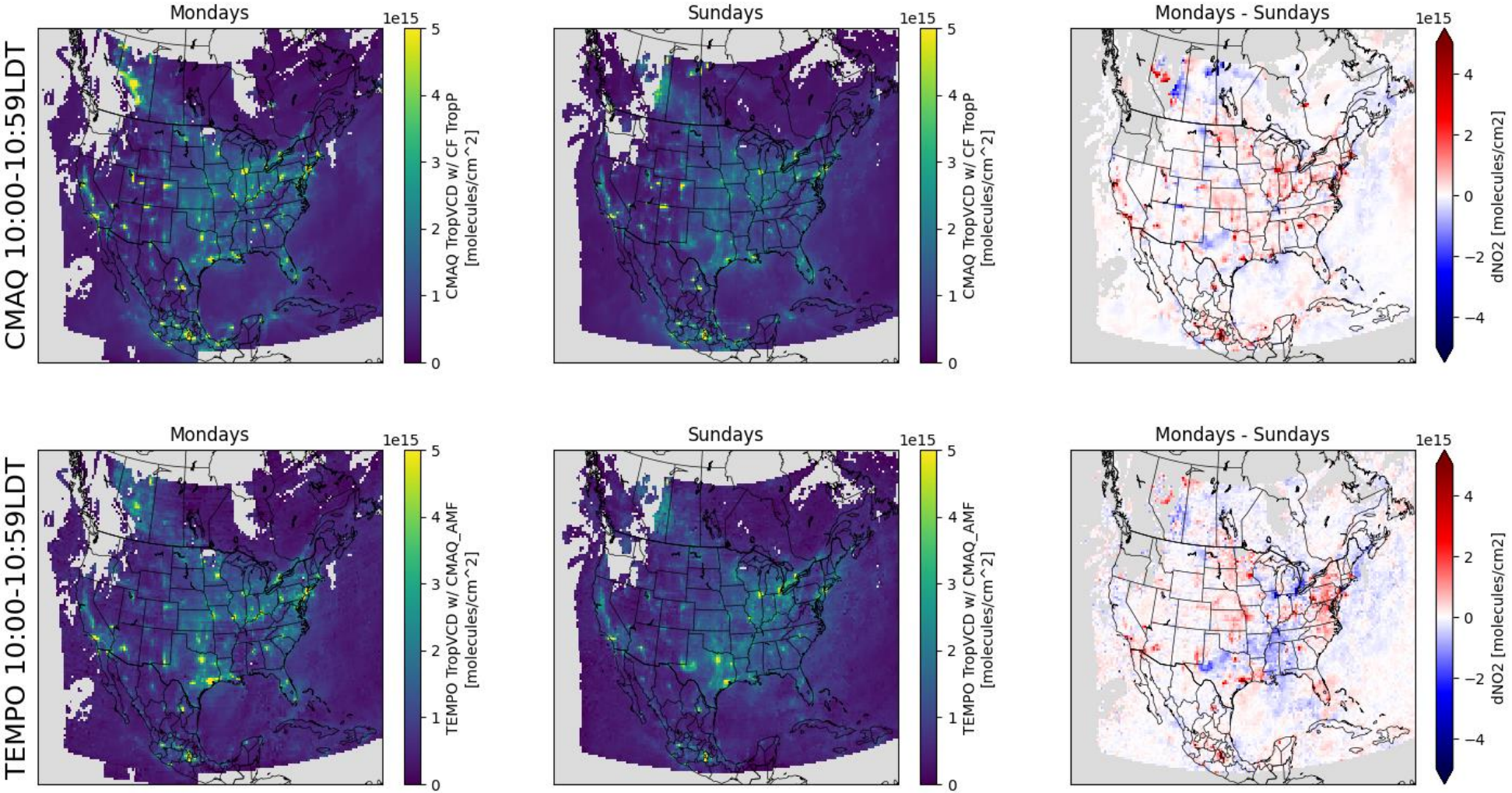
Weekday Increment

1PM overpass

- Weekday/weekend analysis (n=4)
- Tropospheric columns in major cities stand out in both TEMPO and CMAQ
- Mondays larger than Sundays in polluted scenes
- Unexpected differences in Mississippi

Dynamic Evaluation

TEMPO L2 vs Preliminary CMAQ Application



Monday Magnitude | Sunday Magnitude | Weekday Increment

At morning scan

- Weekday/weekend analysis (n=4)
- TEMPO and CMAQ increments over cities are more similar at 10LDT than at 13LDT
- TEMPO has more negative increments than CMAQ in general and over the southeast and Great Lakes in particular.
- TEMPO Chicago increment looks suspect.
- Need longer data to isolate variability vs true difference.

Simple TEMPO Surface NO2

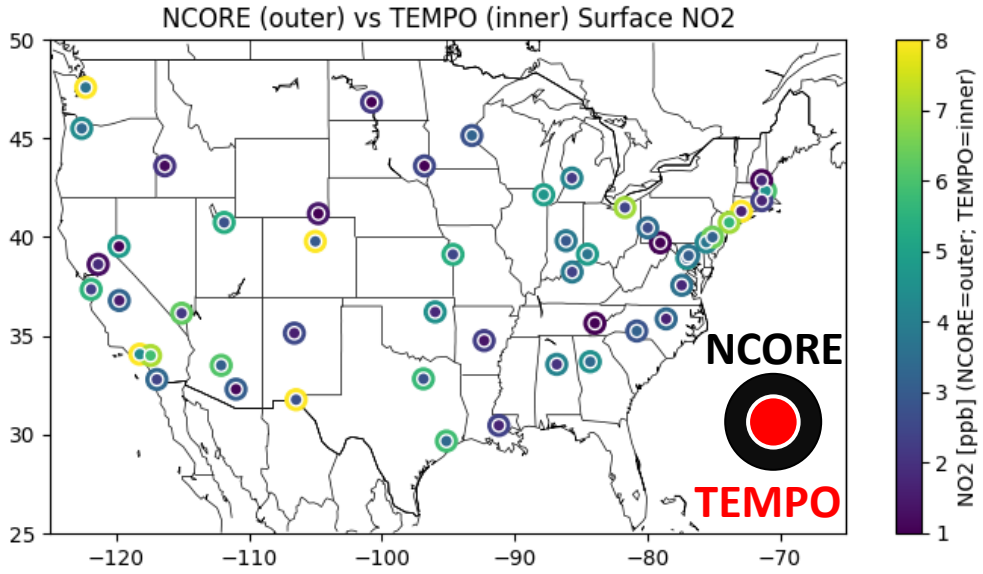
TEMPO L2 vs Preliminary CMAQ Application

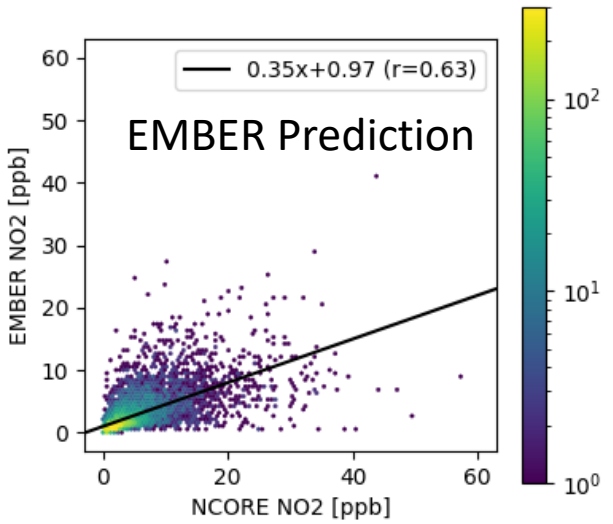
Physical surface NO2 translation from EMBER: $x=\eta\Omega_t$

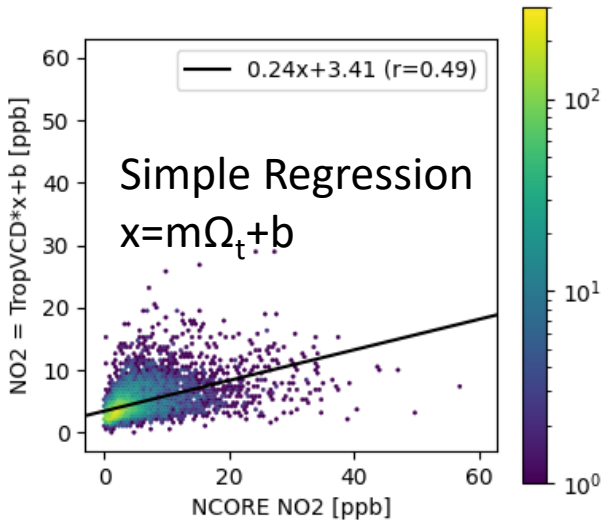
- Surface to tropospheric column from EMBER ($\eta=x_q/\Omega_q$)
- Tropospheric Column from TEMPO (Ω)
- Coarse resolution (36km): exploring NCORE sites only

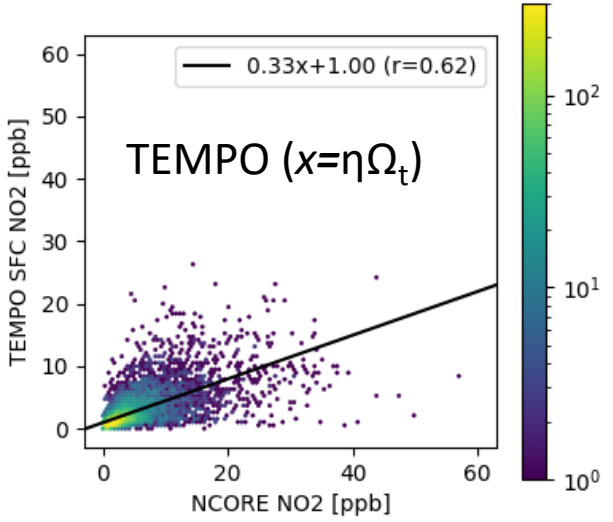
Findings

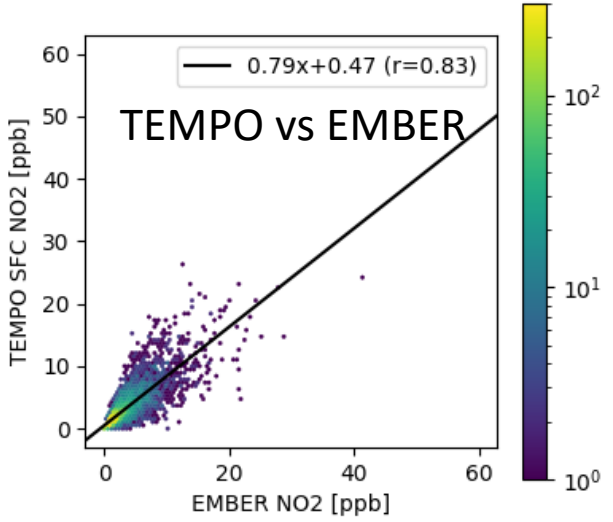
- Physical translation improves on simple regression
- Disagreement in Washington, Colorado and El Paso
- Performance should be enhanced with landuse regression











Summary

- Community led validation TEAM helped TEMPO meet validation goals
  - Nitrogen dioxide and formaldehyde results contribute to both the beta and provisional maturity levels.
  - Assessing bias, precision and uncertainty (NO2-02, NO2-04, HCHO-02 and HCHO-04)
  - Inter-site gradients contributes to urban/rural gradient assessments (NO2-01 and HCHO-01)
  - Large pixel-to-pixel variation and data striping remains
  - Reveals strong disagreement between TEMPO and TropOMI HCHO, which is likely an improvement.
- TEMPO shows 2023 CMAQ simulation low-bias
  - Confirms TropOMI results (Kumm A24A-04 Tue 4:30pm)
  - Geostationary coverage would increase direct assimilation influence on ozone.
- Inferred Surface NO2 shows moderate skill
  - Traditional physical translation improves on simple regression
  - Likely needs additional information from landuse regression to improve (e.g., Anenberg 2022)
- Thanks to:
  - Kelly Chance, SAO, NASA and all the people who helped deliver on the promise of TEMPO!
  - NASA LaRC ASDC for assistance to connect TEMPO to RSIG APIs and increase accessibility!
  - Pandonia Global Network and State and Local agencies for working with EPA to expand Pandora measurements!
  - Research groups and researchers who have contributed their time and analysis in support of TEMPO validation!

email: Henderson.Barron@epa.gov