

NO₂ Algorithm Development for GeoXO ACX



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NO₂ Algorithm for GeoXO ACX

- Direct Vertical Column Fitting (DVCF) Algorithm for NO₂ Retrievals

$$\ln I_m(\lambda) - \ln I_{TOA}(\lambda) = V \int_0^\infty \frac{\partial \ln I_{TOA}(\lambda)}{\partial \tau_z} S_z \sigma(\lambda, T_z) dz - \sum_i^m \xi_i \sigma_i(\lambda, T_i) + \sum_{k=0}^n \frac{\partial \ln I_{TOA}(\lambda)}{\partial R} \Delta R_k (\lambda - \lambda_0)^k + \varepsilon$$

- | | |
|---|--|
| • λ : wavelength | • NO ₂ vertical column : V |
| • I_m : measured radiance | • NO ₂ Shape factor : S_z |
| • I_{TOA} : radiative transfer simulation | • Gas absorber slant columns : ξ_i |
| • σ : gas absorption cross sections | • Aerosol Index : R_1 |
| • R : reflectivity or cloud fraction | • Altitude-resolved AMF: $-\frac{\partial \ln I_{TOA}}{\partial \tau_z}$ |

References:

- Yang et al., 2014, DOI: 10.1002/2014GL060136
 Huang et al., 2022, DOI: 10.1016/j.atmosenv.2022.11936

NO₂ Algorithm for GeoXO ACX

Advanced Algorithm Features

- Allow accurate algorithm physics: explicit treatment of aerosol and surface BRDF to provide accurate representation of spectral and altitude variations of measurement sensitivities (DOAS's equivalent is the improved AMF).
- Allow more accurate stratosphere-troposphere separation by combining retrievals from UV and VIS spectra
- Allow soft calibration to correct biases in radiometric calibration and instrumental features that interfere with the interpretation of molecular absorptions.

Applications to GEMS and TEMPO

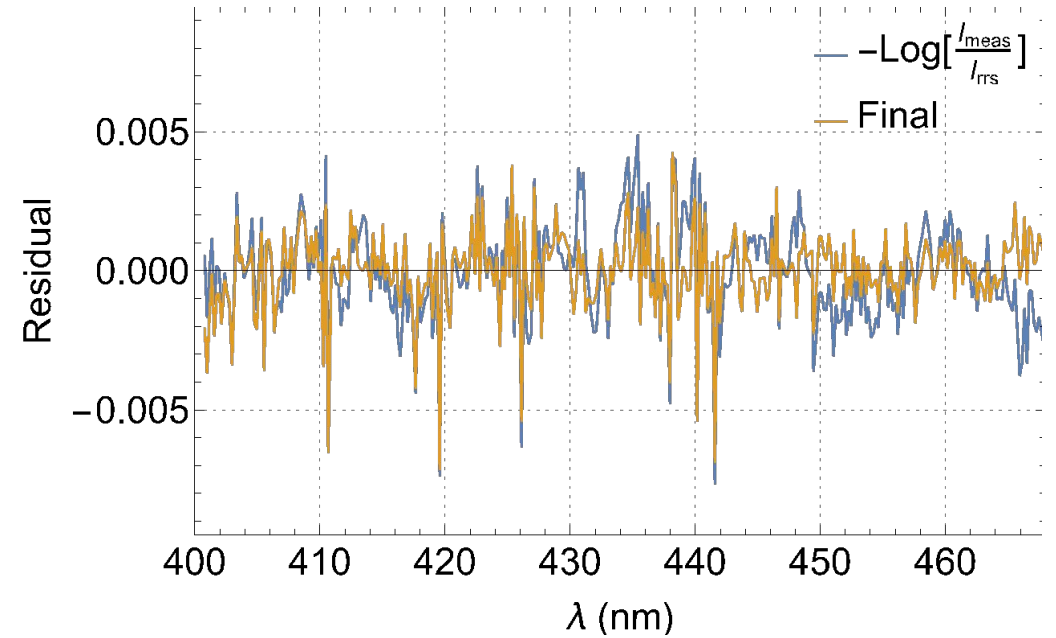
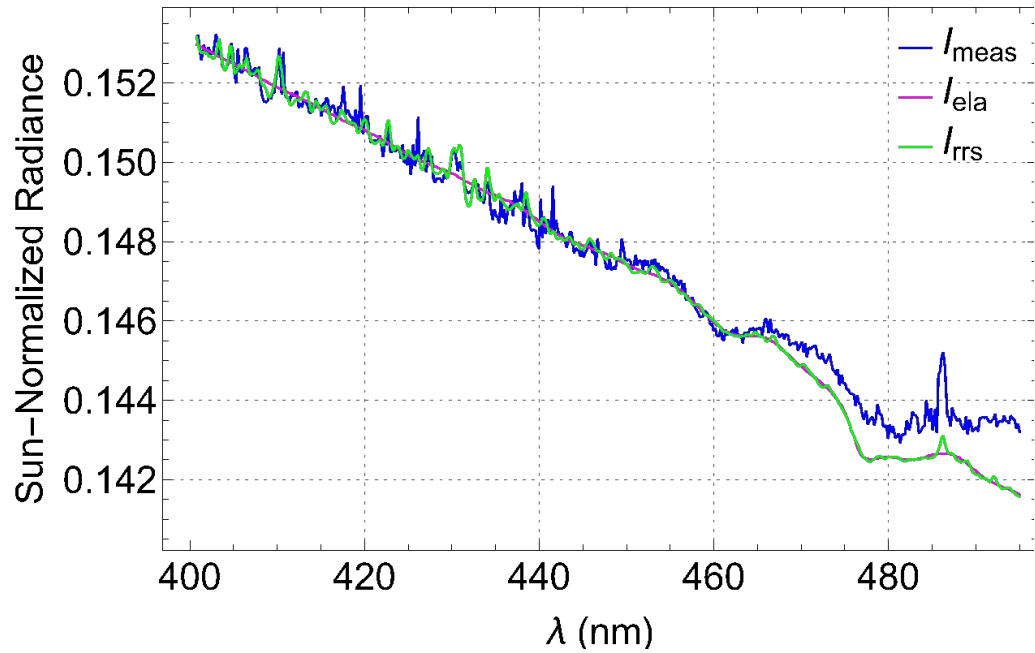
- In preparation for GeoXO ACX, we apply the ACX NO₂ (DVCF) algorithm to proxy data to develop and perfect techniques for handling measurement characteristics:
 - wavelength registrations
 - instrument spectral responses
 - anomalous pixels
 - calibration biases
 - common mode spectra
- Demonstrate accurate and precise retrievals from measurements with various imperfections

Proxy Data



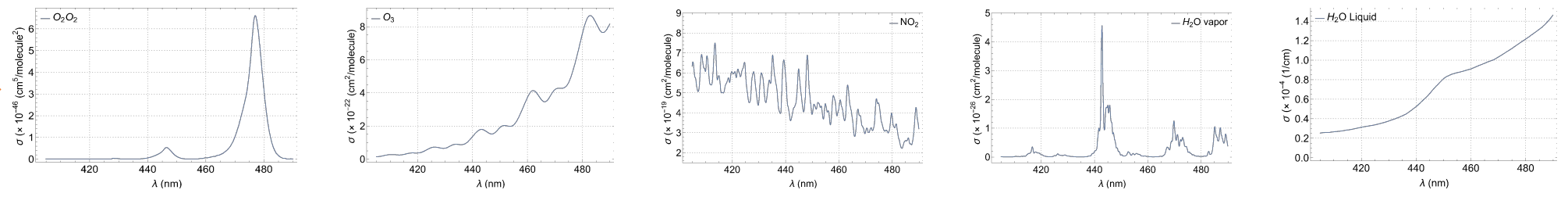
We acknowledge the L1 data providers: US TEMPO team and South Korea's NIER.

Illustration of ACX NO₂ Retrieval

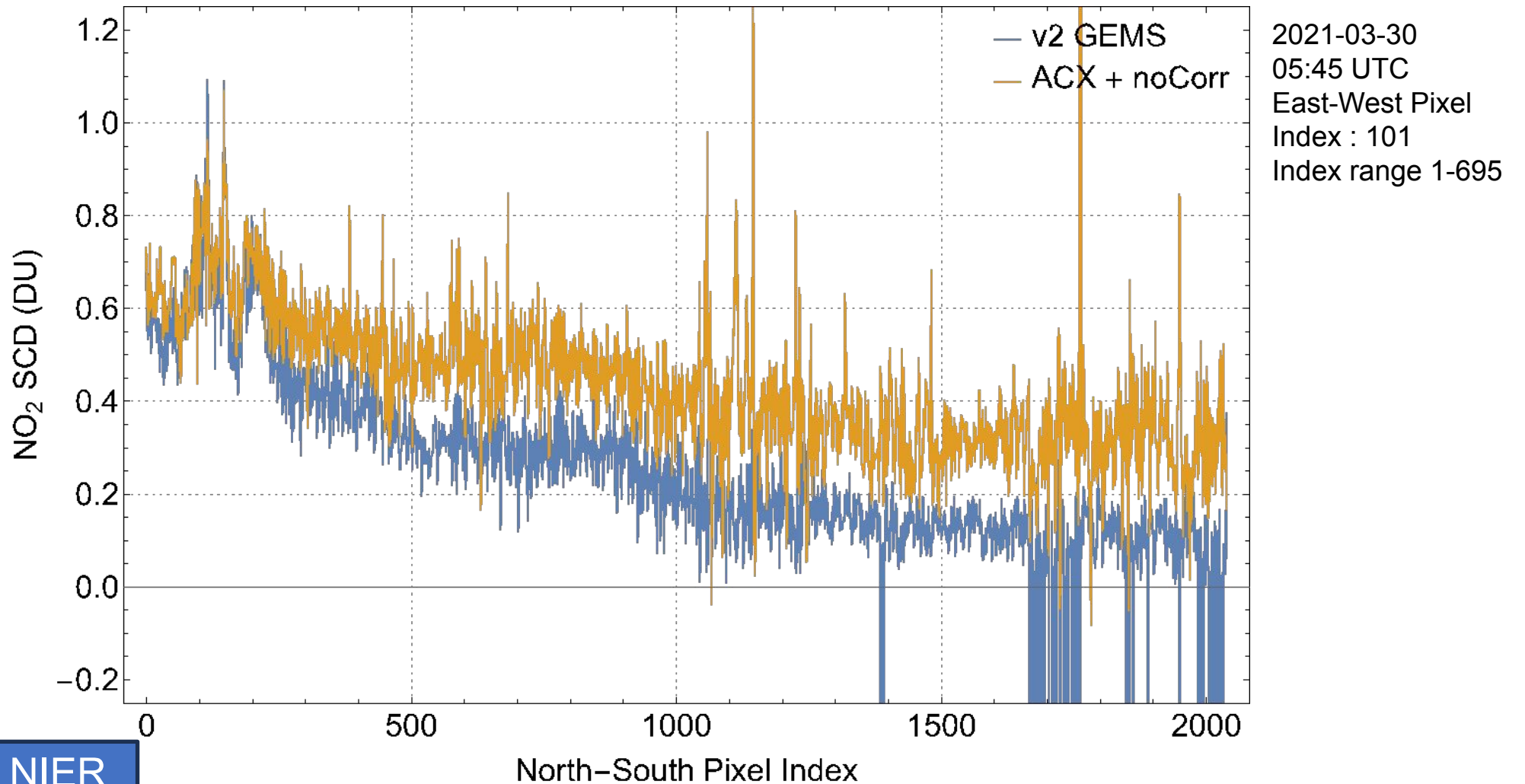


- Information + error are contained in spectral residual: $-\text{Log}[I_{meas}/I_{rrs}]$
- Fitting of residual with reference spectra to extract slant (or vertical) columns

reference spectra

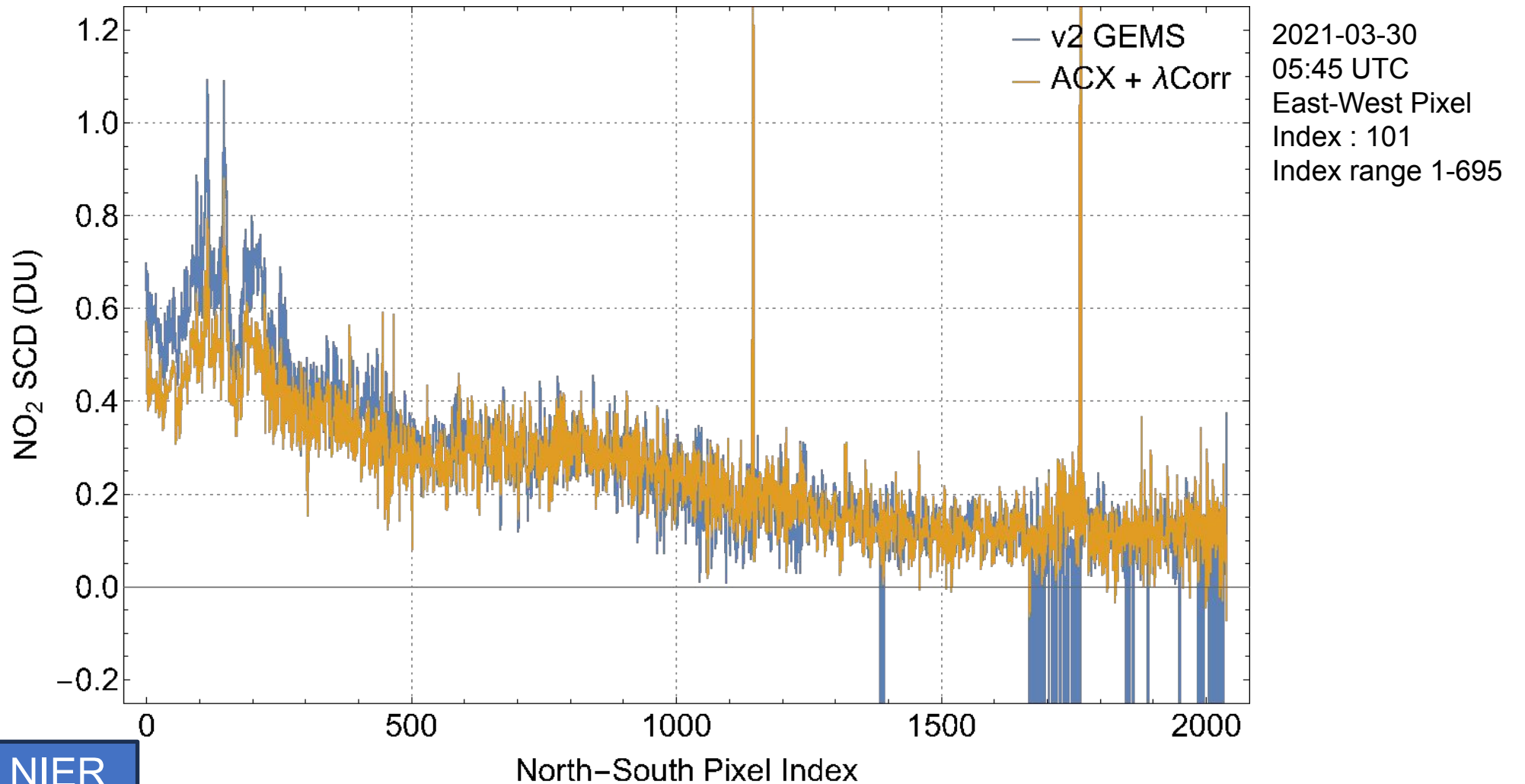


Comparison of GEMS Slant Columns: v2 GEMS vs ACX Algorithm



V2 GEMS is from NIER

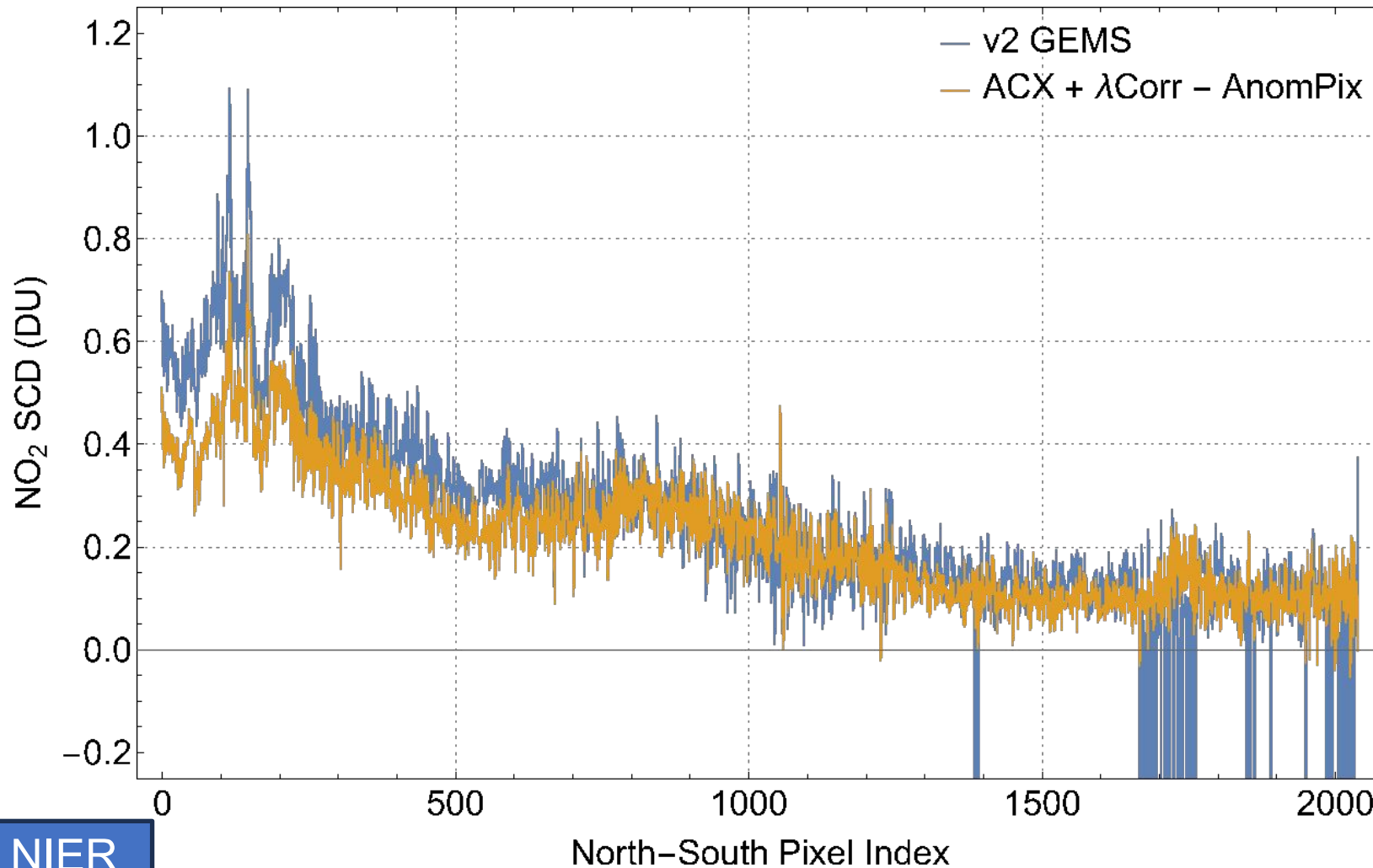
Comparison of GEMS Slant Columns: v2 GEMS vs ACX Algorithm



V1 GEMS is from NIER



Comparison of GEMS Slant Columns: v2 GEMS vs ACX Algorithm



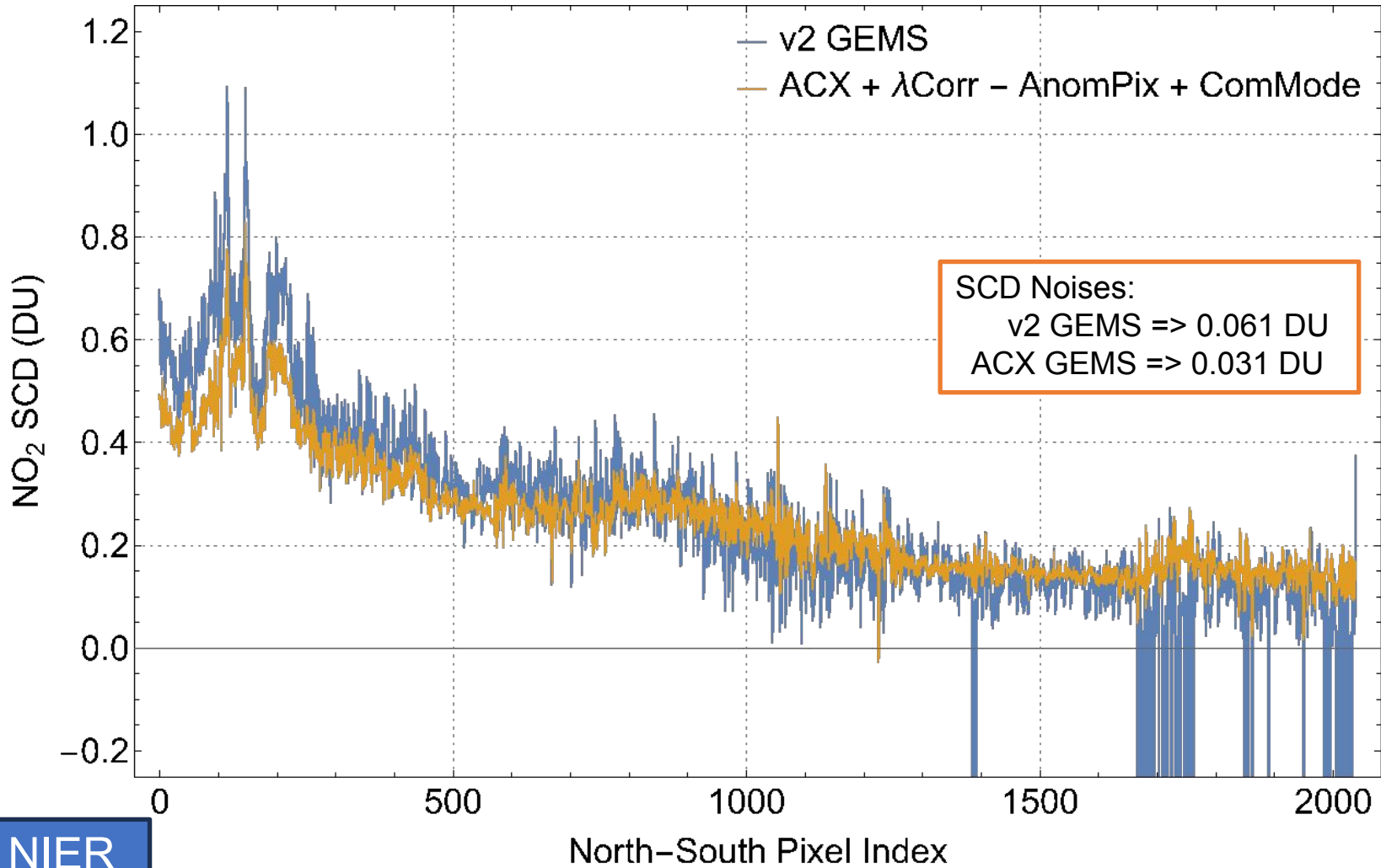
2021-03-30
05:45 UTC
East-West Pixel
Index : 101
Index range 1-695

V1 GEMS is from NIER

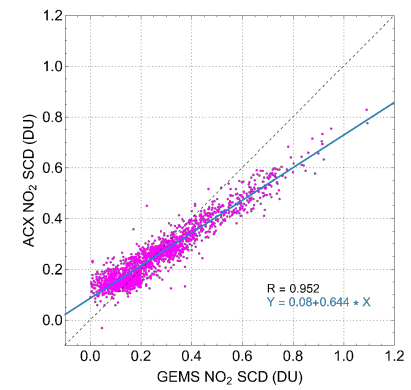


Comparison of GEMS Slant Columns: v2 GEMS vs ACX Algorithm

Precision improvements means more reliable detections of small NO₂ variations, especially important for regions with low pollution levels, e.g., over US.



2021-03-30
05:45 UTC
East-West Pixel Index : 101
Index range 1-695



V2 GEMS is from NIER



Intercomparisons of Slant Columns: TROPOMI vs GEMS and vs TEMPO

A retrieval algorithm may be separated into two parts

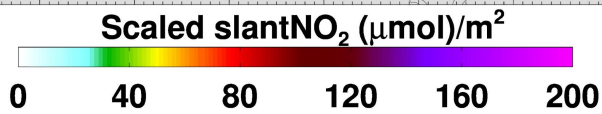
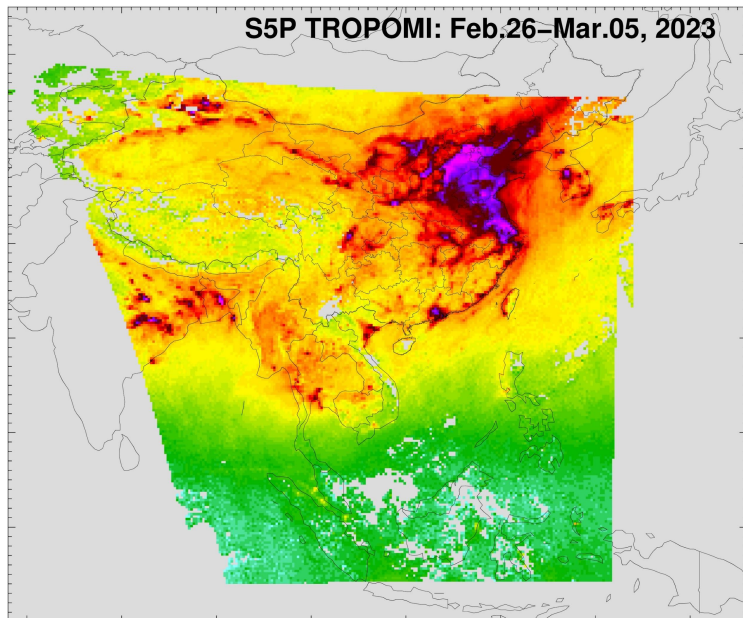
1. Information content quantification => retrieve slant columns
2. Interpretation of Information content => derive vertical columns
 - Slant columns are independent of retrieval assumptions of vertical profiles, surface reflections, and clouds/aerosols, while vertical columns depends on their proper treatments.
 - Slant columns are geometry dependent

Sample selection for NO₂ Slant Column Comparisons

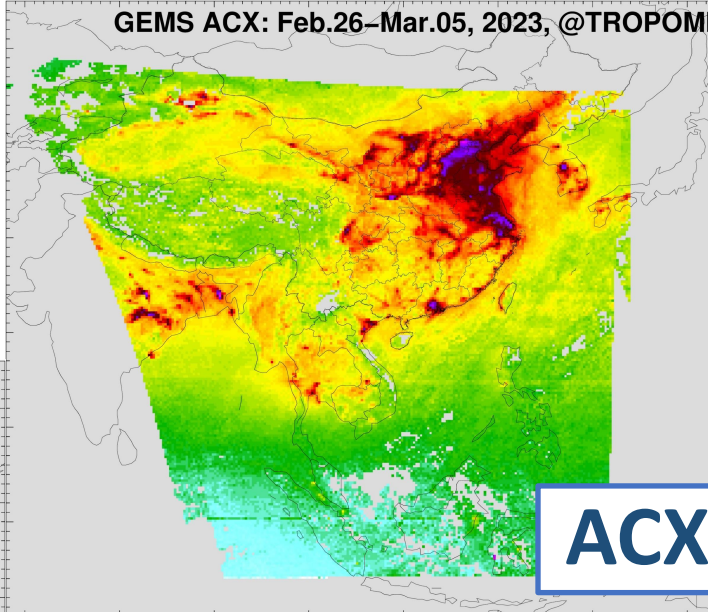
- Near-coincident: same grid cells (0.25° X 0.25°) and ± 30 minutes
- Slant columns are divided by geometric air mass factors (AMF_G) to reduce the impact of path-length difference
- Cloud fraction < 0.2

$$AMF_G = 1/\text{Cos}[VZA] + 1/\text{Cos}[SZA]$$

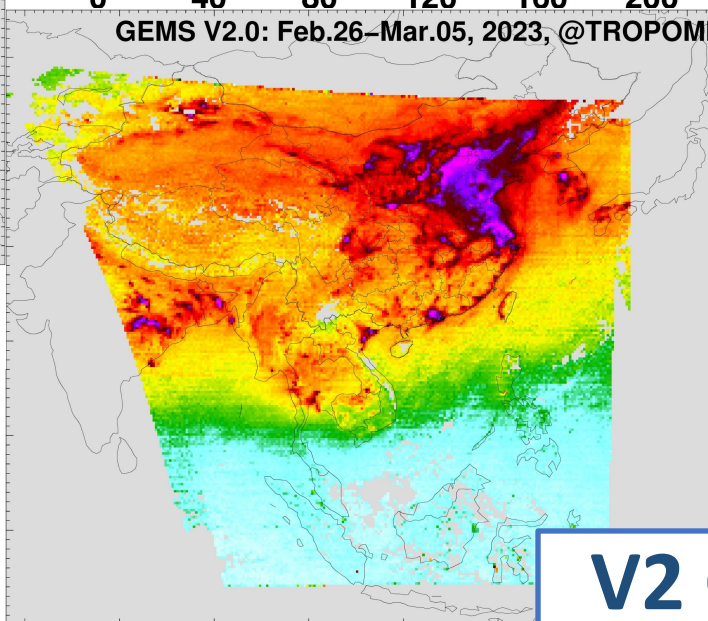
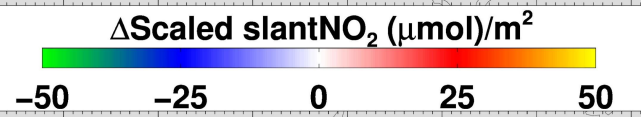
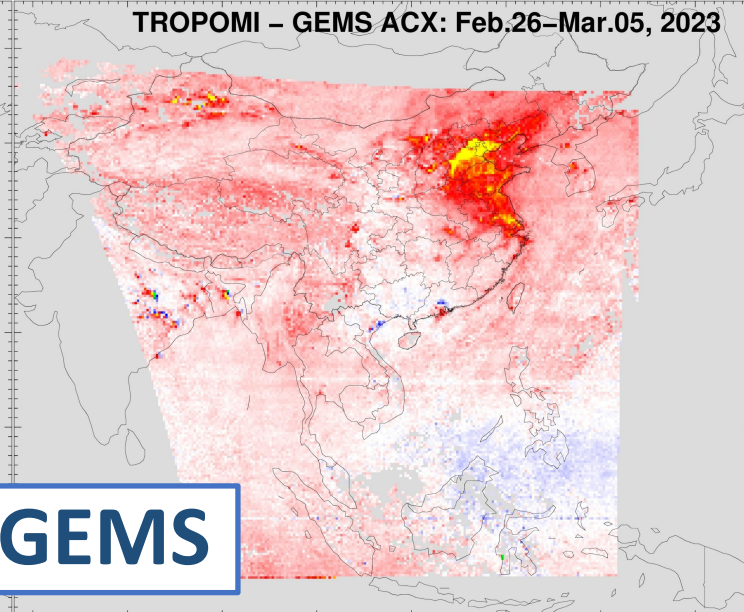
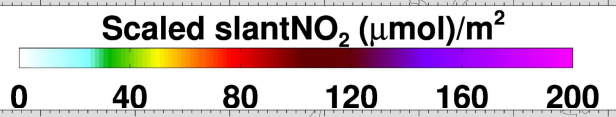
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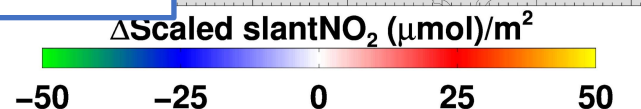
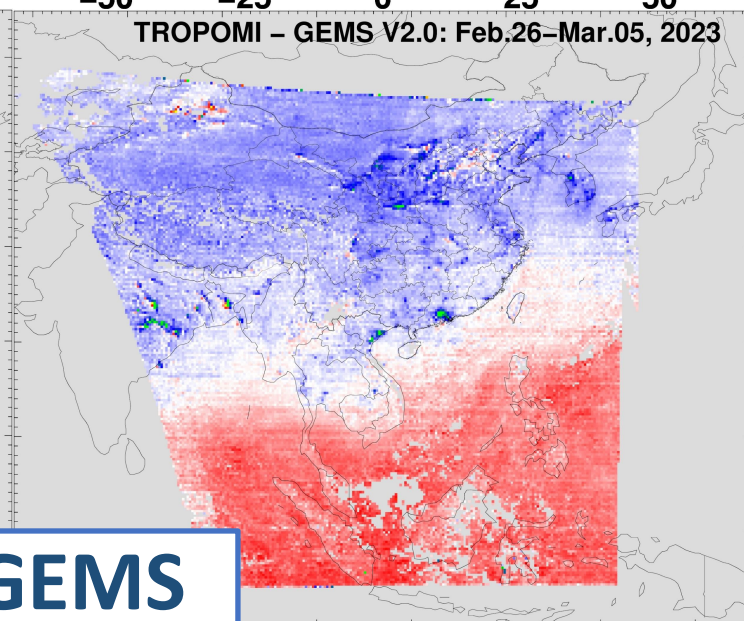
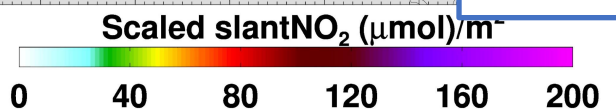
TROPOMI



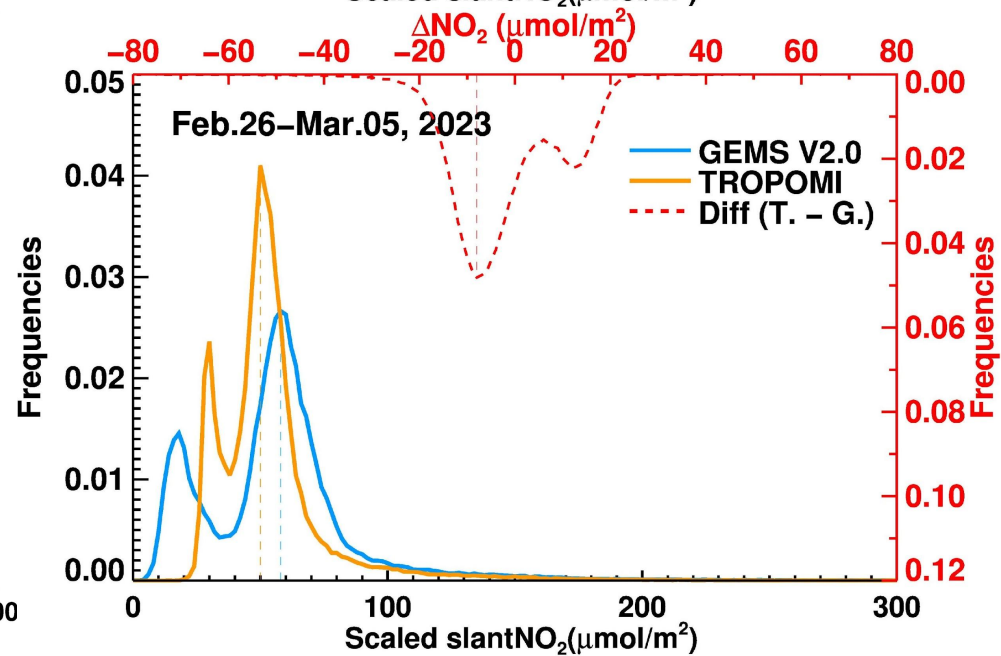
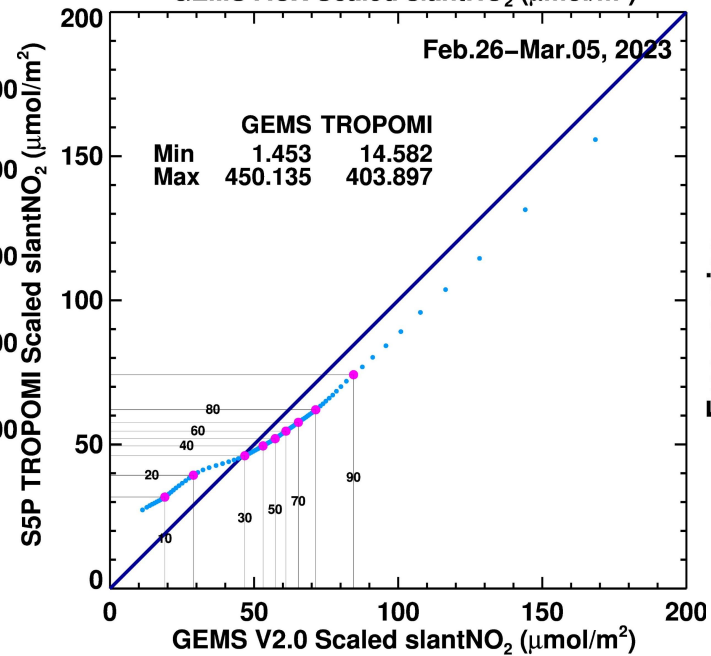
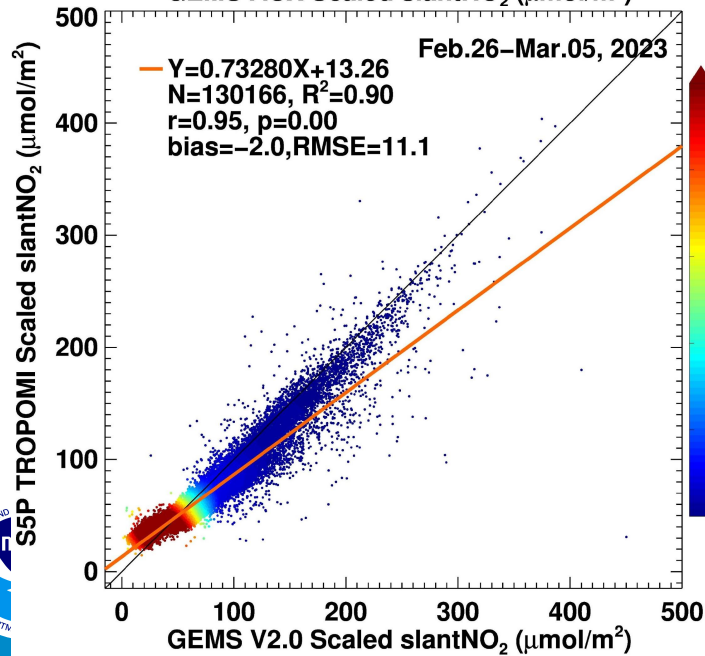
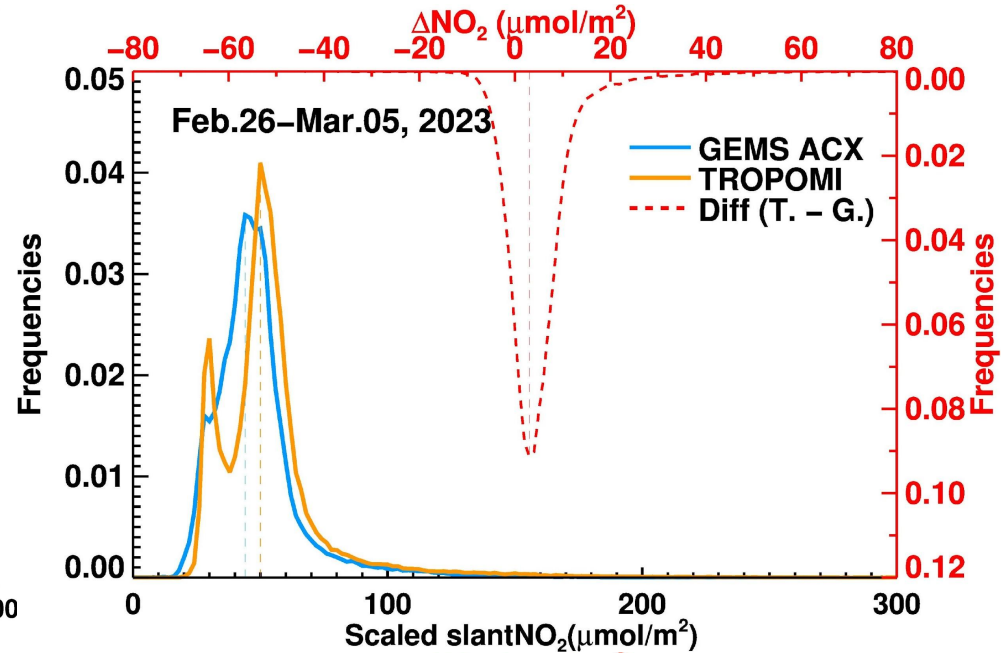
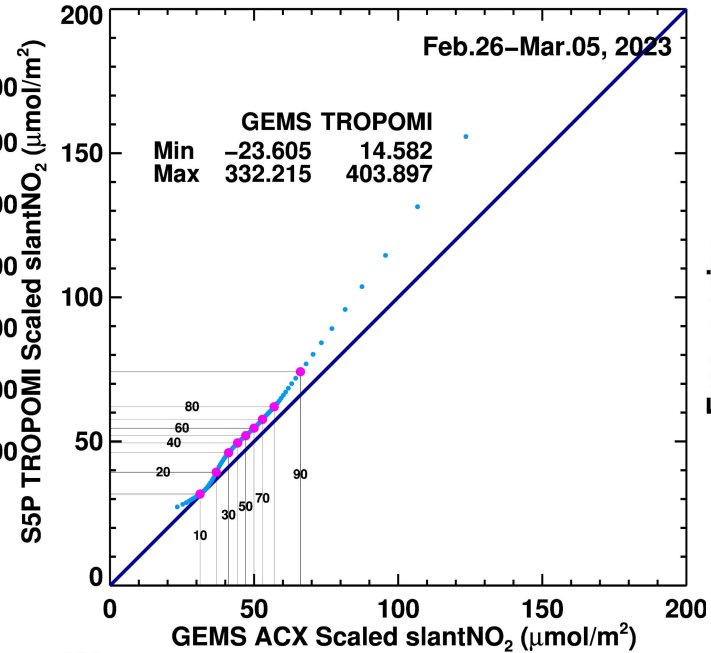
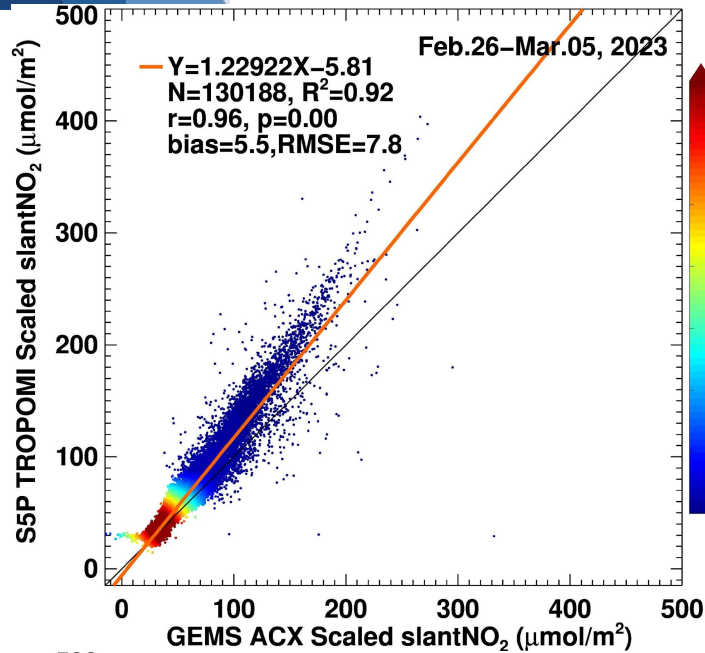
ACX GEMS



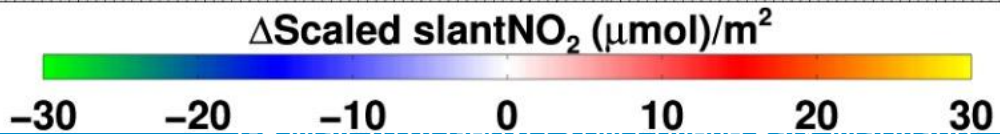
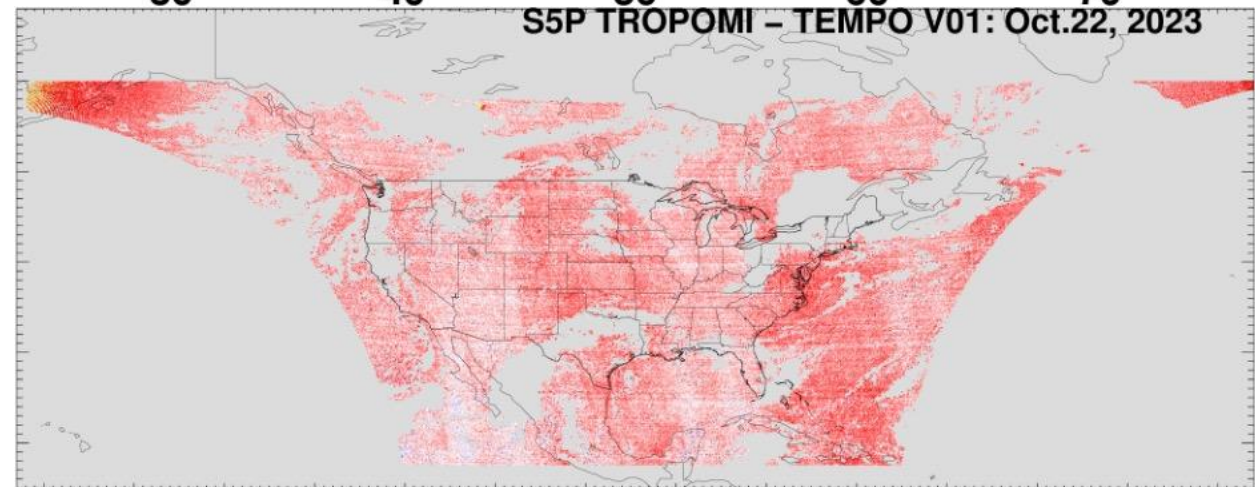
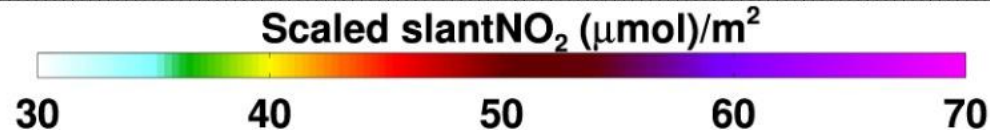
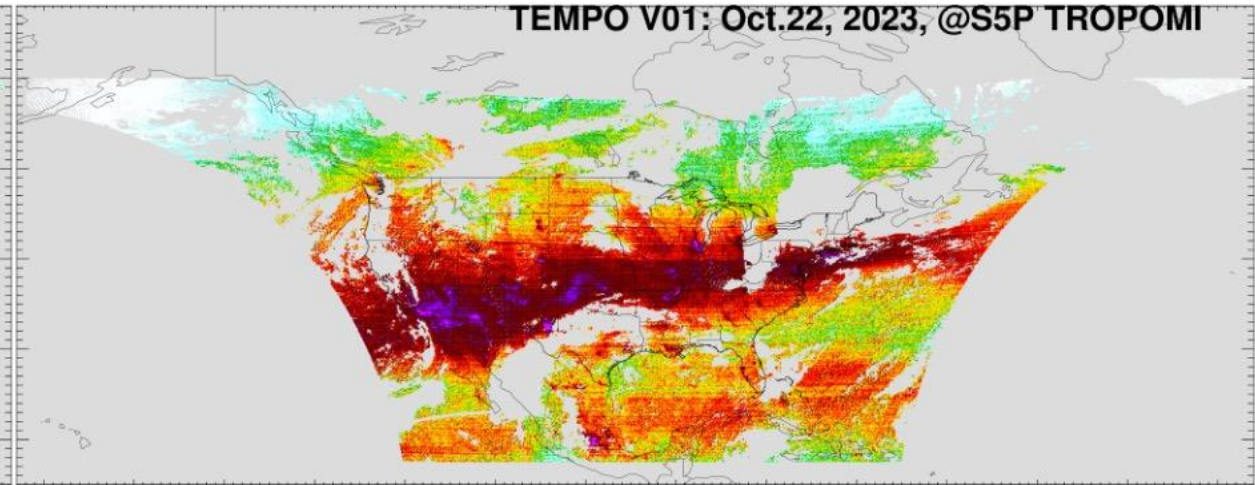
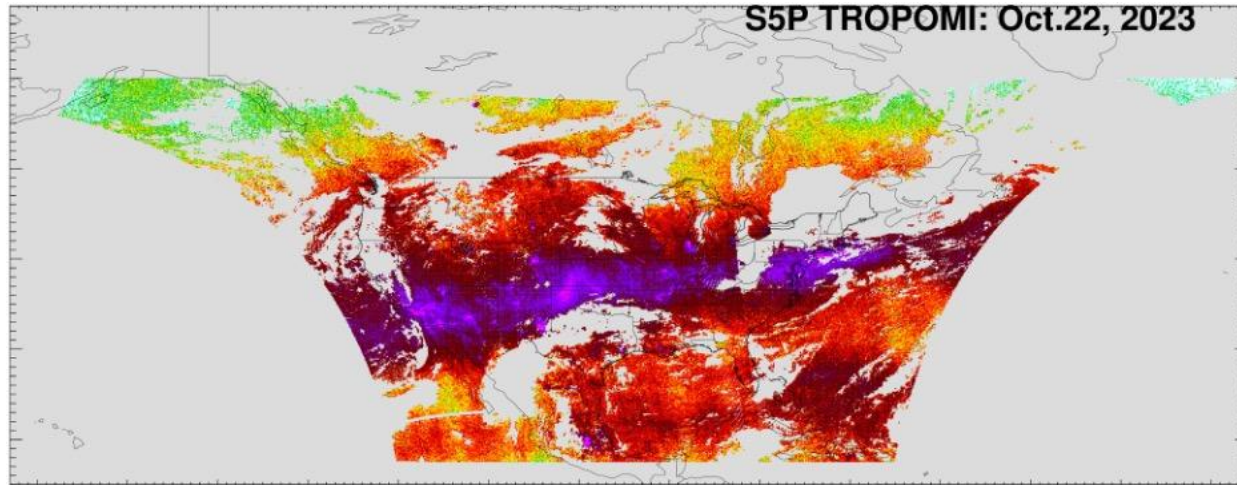
V2 GEMS



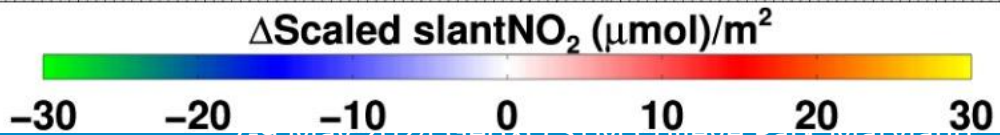
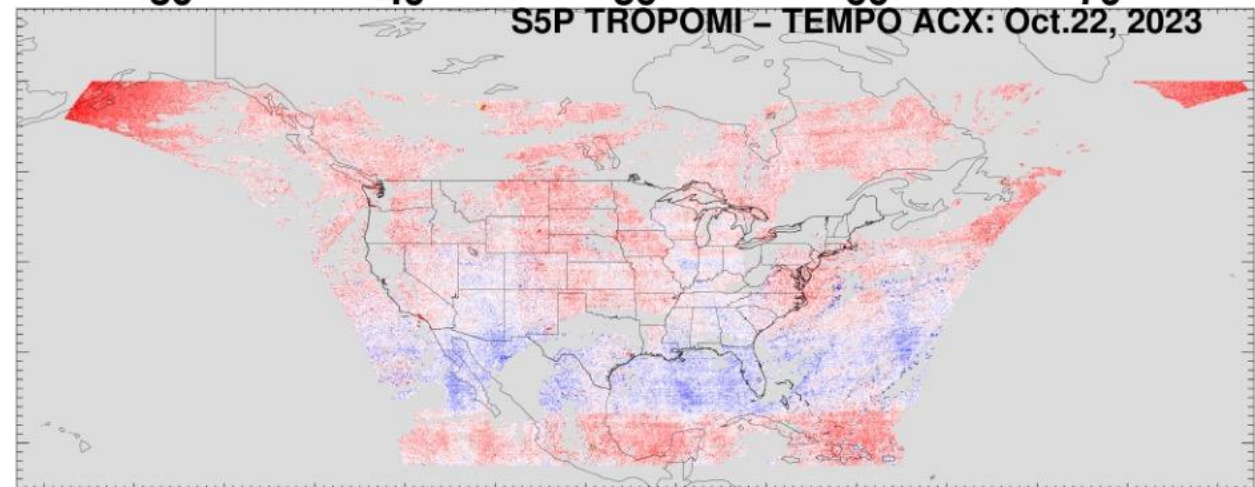
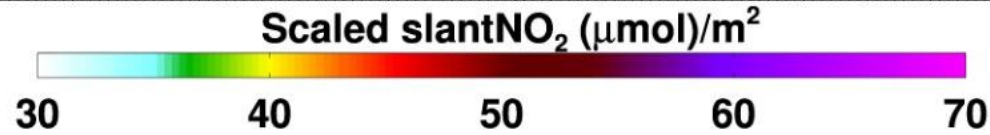
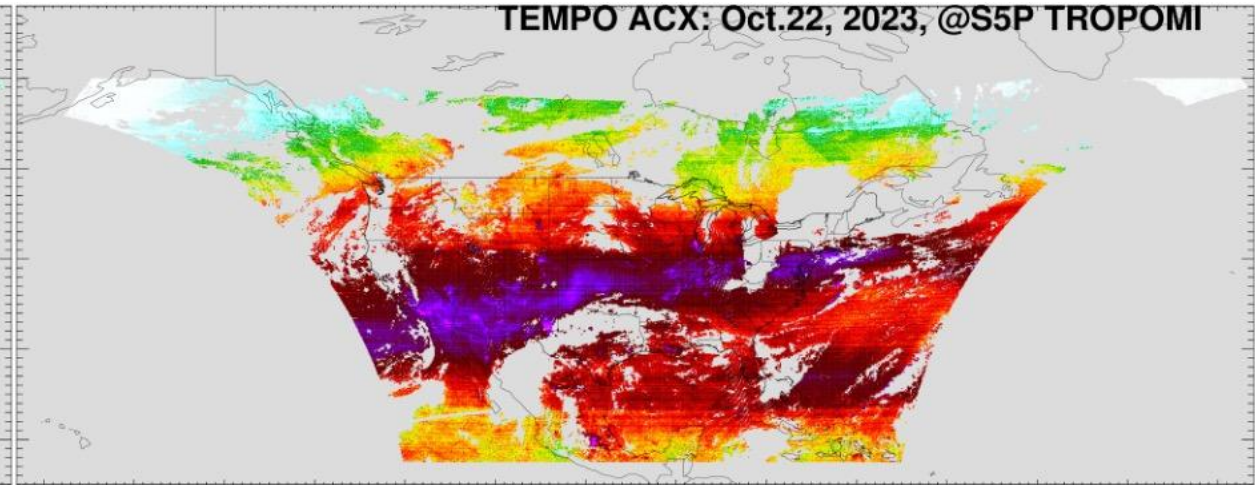
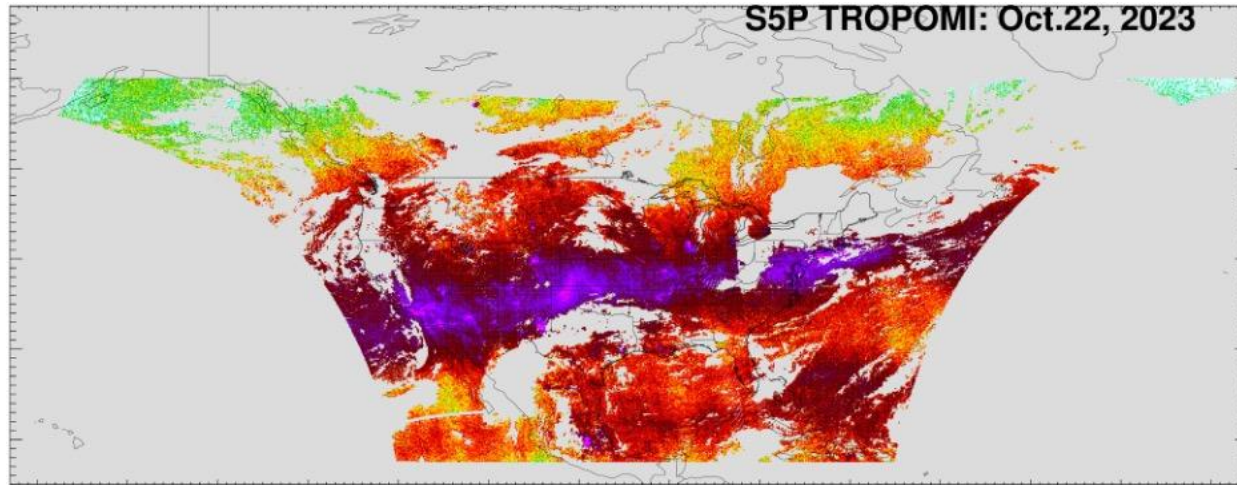
TROPOMI vs ACX and V2 GEMS



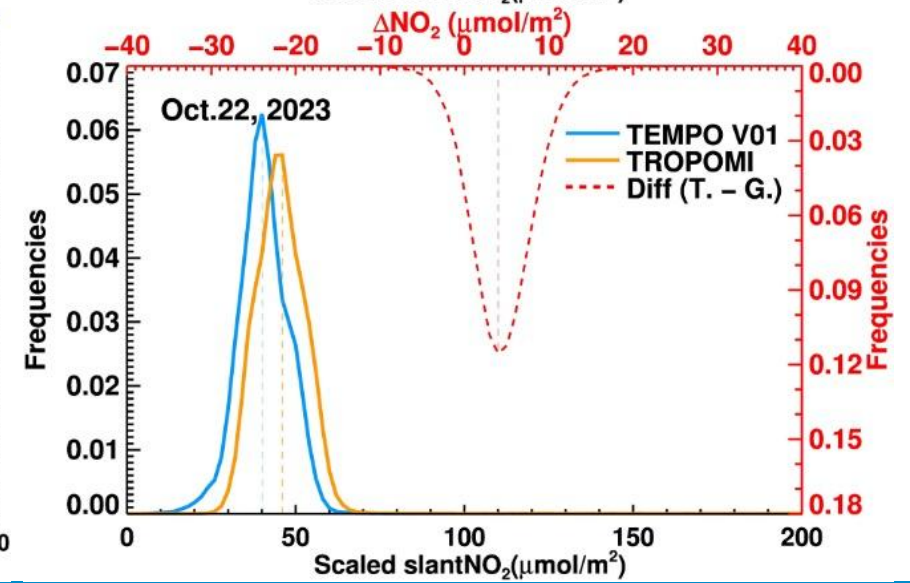
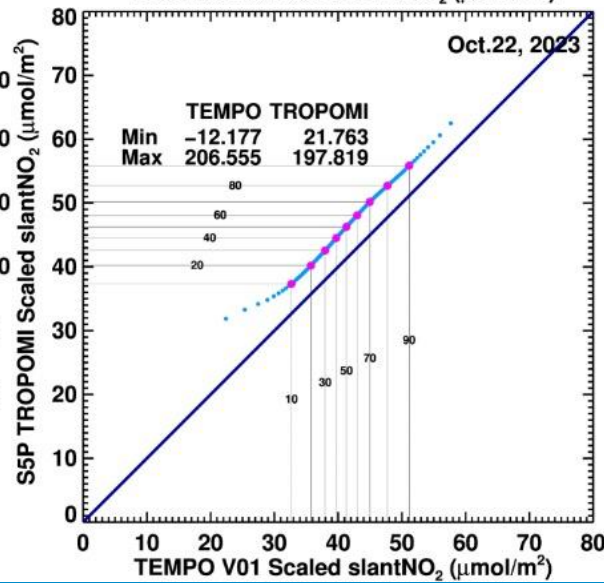
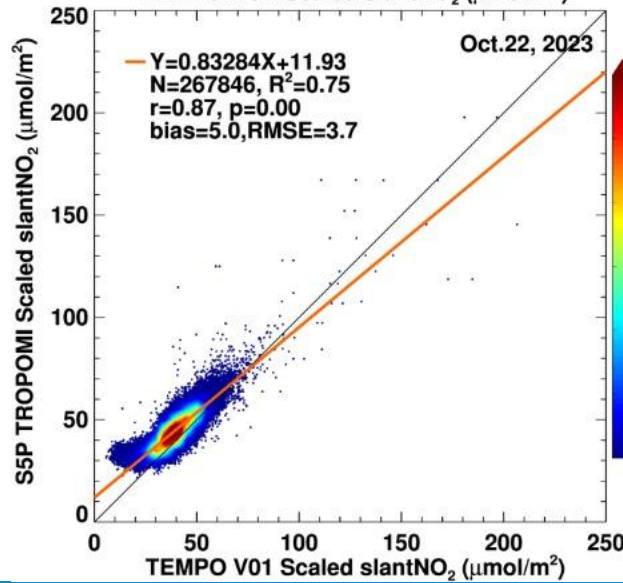
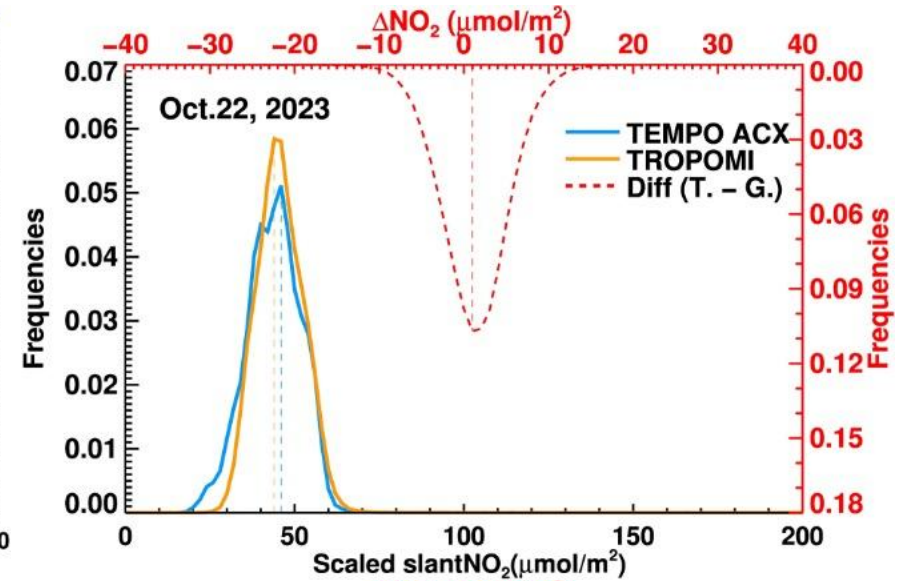
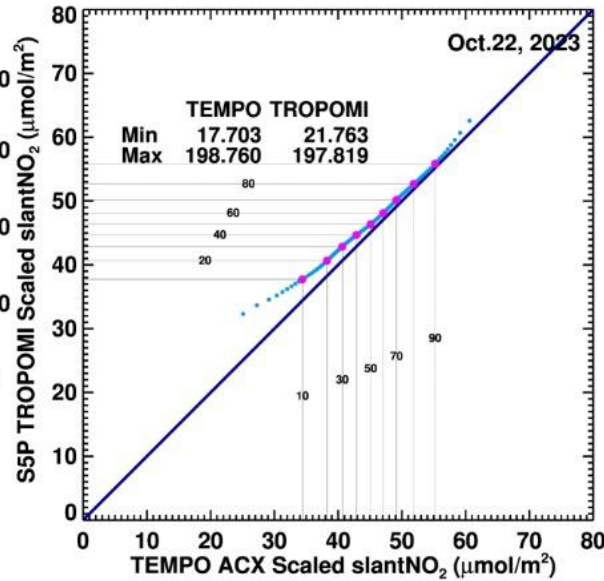
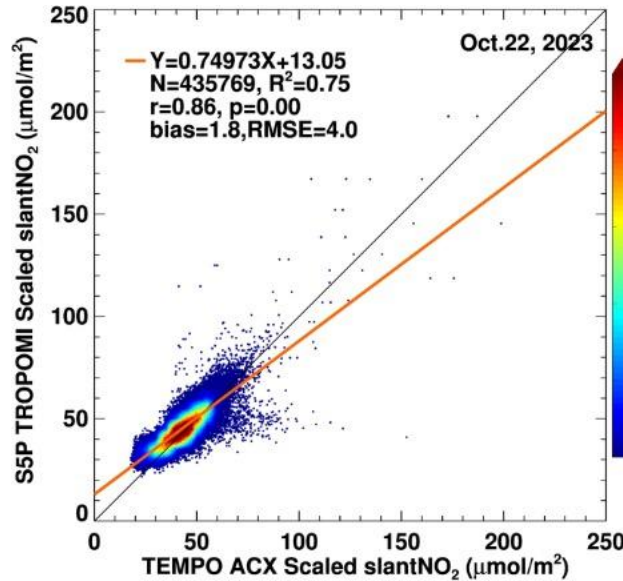
TROPOMI vs V1 TEMPO



TROPOMI vs ACX TEMPO



TROPOMI vs ACX and V1 TEMPO

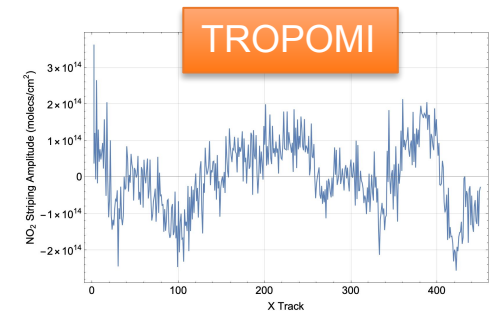


Comparison Summary

- Systematic biases of scaled slant NO₂ columns
 - TROPOMI > ACX TEMPO > v1 TEMPO
 - TROPOMI > ACX GEMS
 - TROPOMI < v2 GEMS at northern latitudes
 - TROPOMI > v2 GEMS at southern latitudes
- ACX TEMPO and ACX GEMS are consistent: bias low similarly against TROPOMI

Source of Biases

- Systematic biases likely originate from persistent spectral patterns in the sun-normalized radiance spectra, which usually correlate with a molecular absorption spectrum, resulting in biases in the slant columns.
- **Corrections** (detector dependent)
 - **TROPOMI** -> Across-track NO_2 slant column stripe offset, 7-day mean, determined over the Pacific Ocean
 - **ACX algorithm** -> removing common mode spectra derived from residuals over areas with small (< 0.05 DU) tropospheric NO_2 columns.

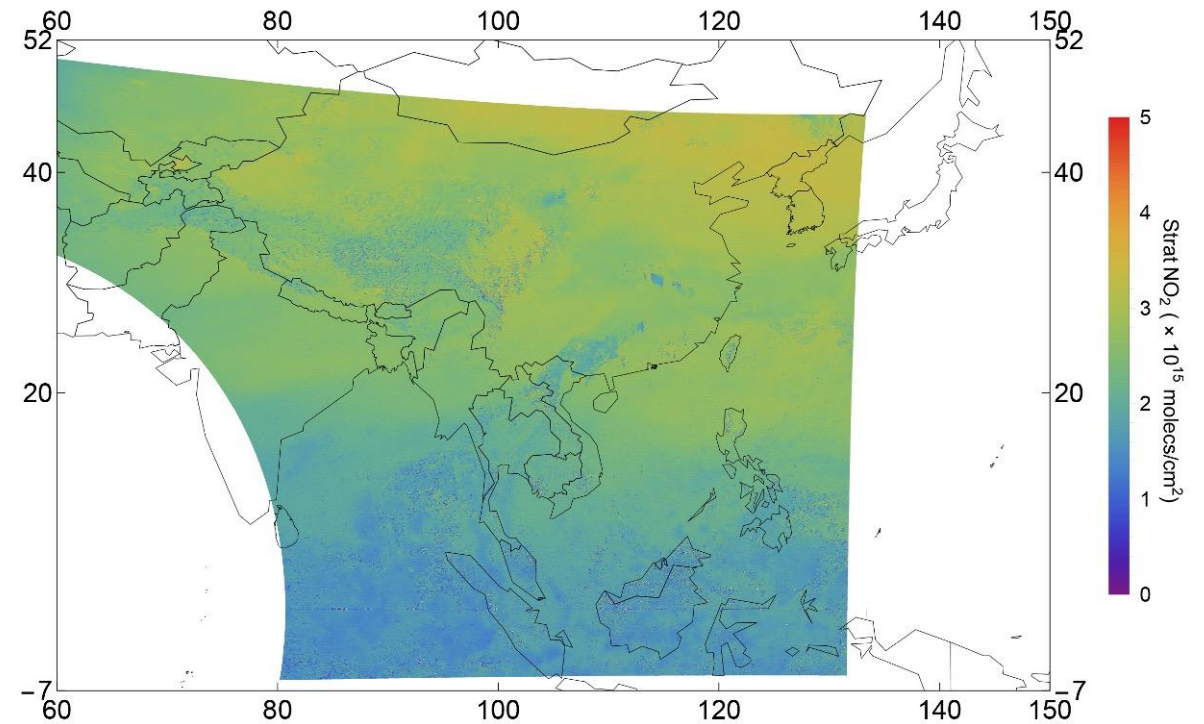
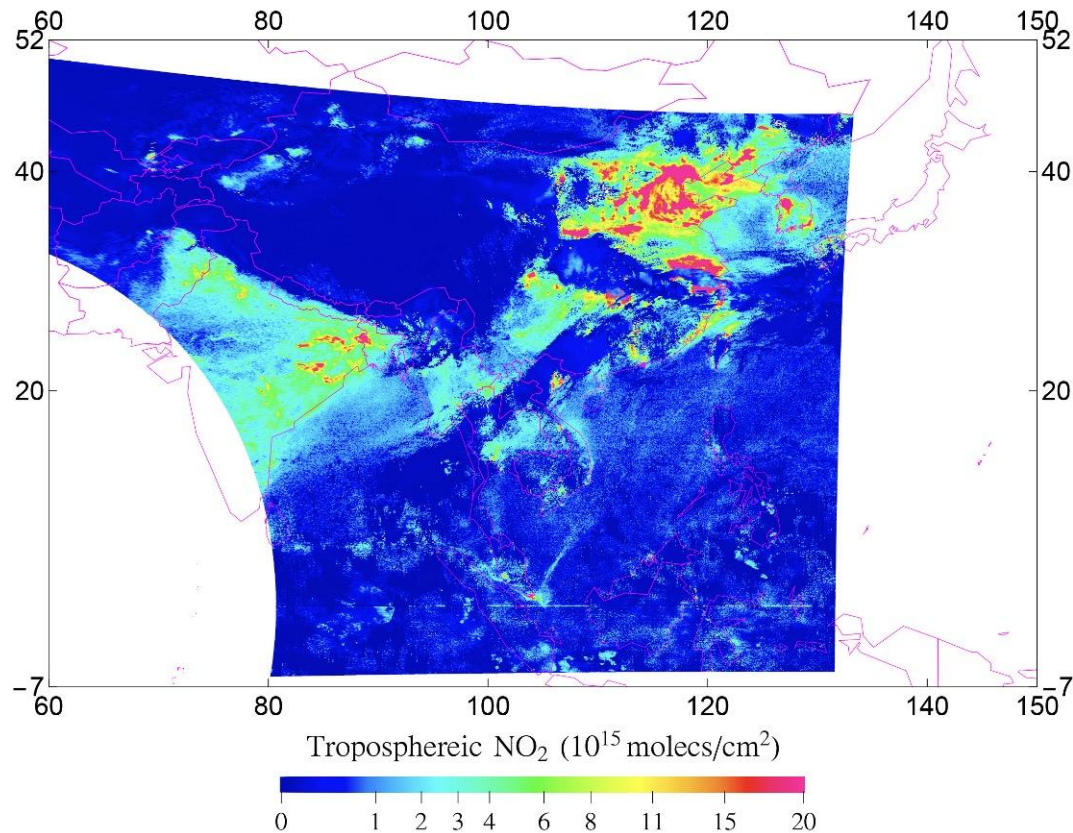


Radiance space corrections work for OMI, OMPS, TROPOMI, GEMS, TEMPO.

ACX Algorithm on GEMS 2021-03-30_0045

Tropospheric NO₂

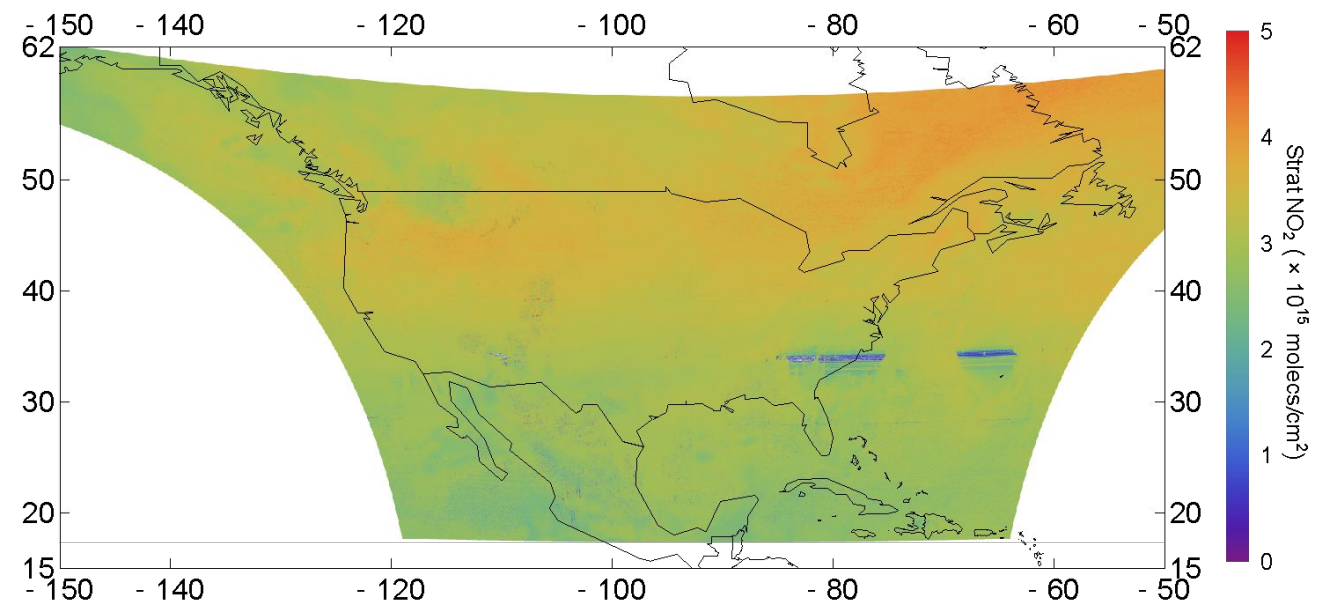
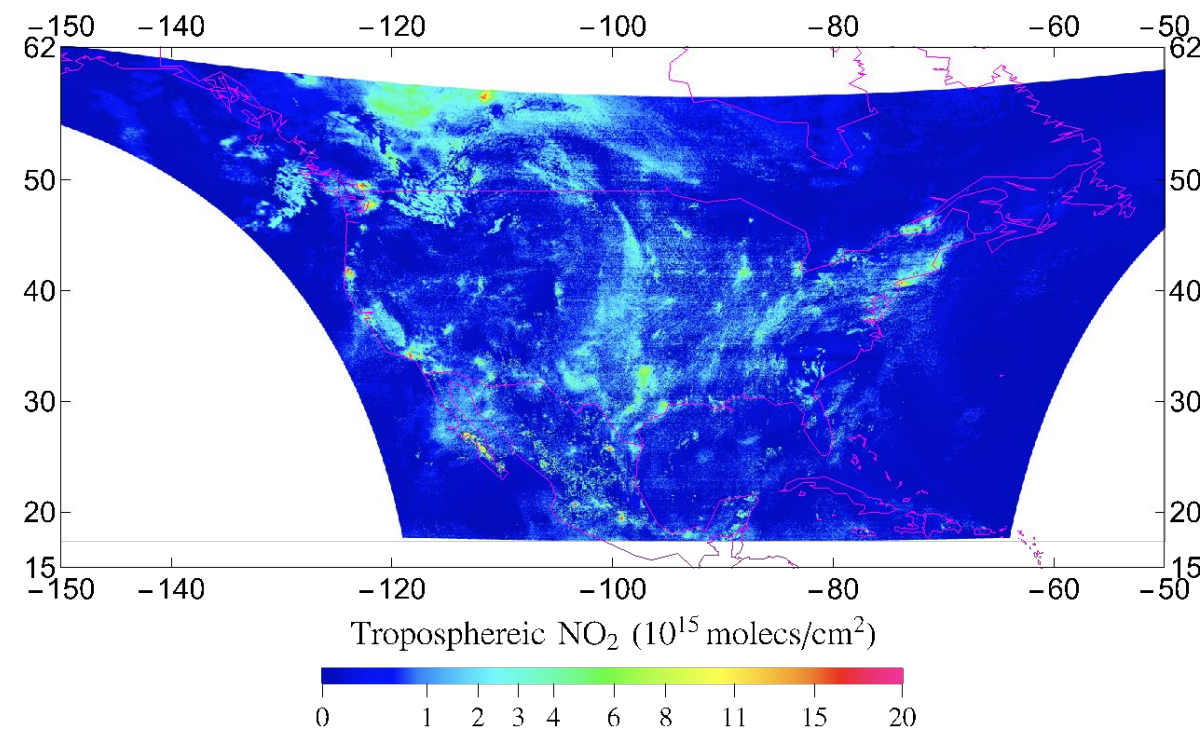
Stratospheric NO₂



ACX Algorithm on TEMPO 2023-08-30-S010

Tropospheric NO₂

Stratospheric NO₂



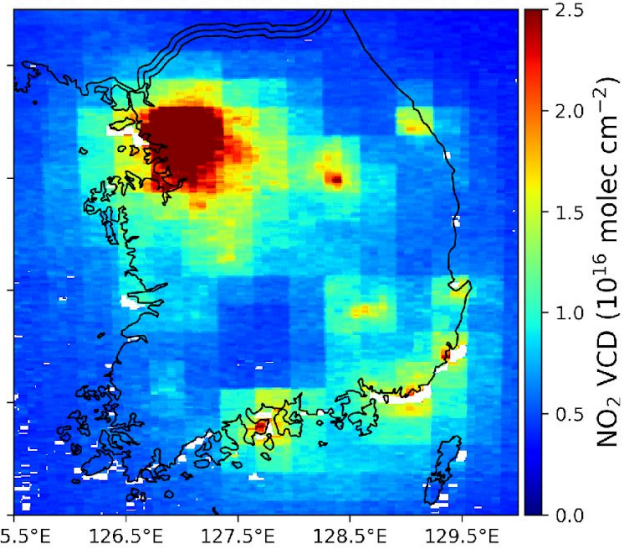
Summary

- Applications of the ACX NO₂ algorithm to GEMS and TEMPO yield high-quality (i.e., low noise, few artifacts, and high accuracy) NO₂ products. ACX NO₂ achieved lower noise levels than the corresponding standard products.
- Demonstrate the capability of rapid (near-real-time) production of high quality NO₂ data soon after ACX starts Earth observation

Intercomparisons of Tropospheric NO₂ Monthly Means for October 2021

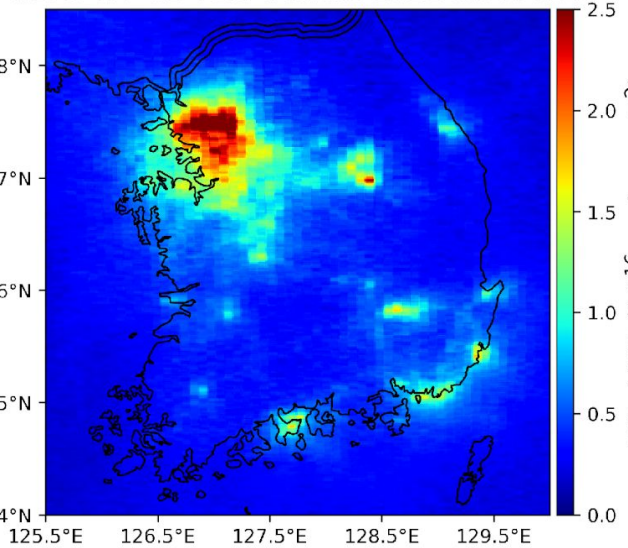
GEMS Standard Product

GEMS L2 v2.0 October 2021 13:45 KST



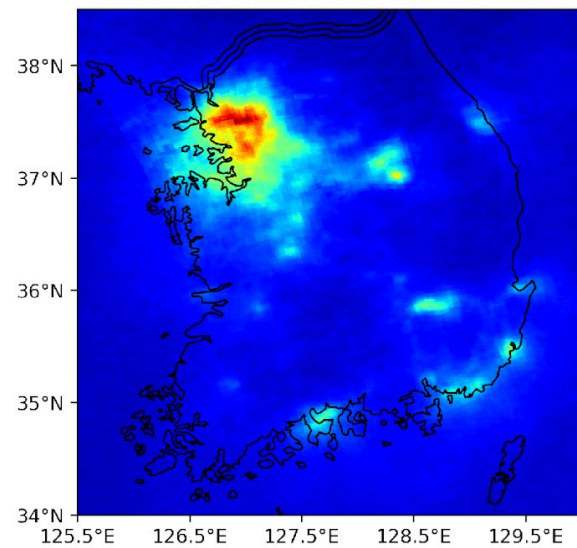
GEMS IUP-UB

GEMS IUP-UB v1.0 October 2021 13:45 KST

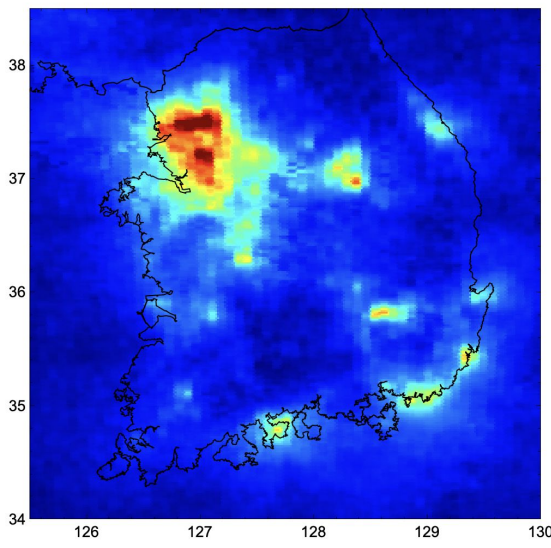


TROPOMI

TROPOMI V02.04.00 October 2021



GEMS ACX



Left 3 panels are copied from
<https://doi.org/10.5194/egusphere-2024-6>

Plan

- Algorithm physics improvements: surface reflection (BRDF), aerosol/cloud treatments
- Implementation of joint UV and visible retrievals for NO₂ stratosphere-troposphere separation
- Extensive comparisons and validations to verify the ACX NO₂ accuracy and quantify its uncertainties

Acknowledgement

- We thank the TEMPO science team and the NIER (South Korea's National Institute of Environmental Research) for providing L1 data used in our algorithm development.