

Tropospheric Emissions:
Monitoring of Pollution



A New Era of Air Quality Monitoring from Space over North America with TEMPO: Commissioning and Early Nominal Operation Results

Xiong Liu¹, Kelly Chance¹, Raid Suleiman¹, John Houck¹, John Davis¹

Kevin Daugherty², David Flittner², David Rosenbaum², Crystal Fenn²

Gonzalo Gonzalez Abad¹, Caroline Nowlan¹, Huiqun Wang¹, Heesung Chong¹,

Weizhen Hou¹, Junsung Park¹, Christopher Chan Miller¹, Juseon Bak¹, Jim Carr,

James Szykman, Mike Newchurch, Aaron Naeger, Ronald Cohen, Zolal Ayazpour¹,

Christopher Brown², Zachary Fasnacht, Marcellin Feasson¹, Jean Fitzmaurice¹,

Jeffrey Geddes, David Haffner, Jay Herman, Joanna Joiner, Laura Judd,

Emma Knowland, Xuming Lei, Nischal Mishra², Robert Neece², Ewan O'Sullivan¹,

Brad Pierce, Wenhan Qin, Eric Roback², Justin Strickland², Robert Spurr,

Luke Valin, Alexander Vasilkov, Eun-Su Yang, Barron Henderson,

Katherine Travis, Prajjwal Rawat, and the TEMPO Team

¹CfA | Harvard & Smithsonian

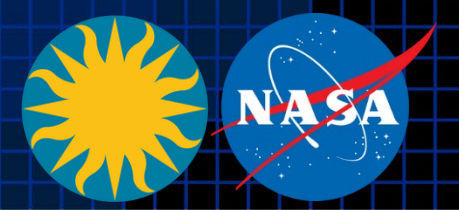
Int'l. Space Science Institute (ISSI) Workshop on
Geostationary Satellites & Atmospheric Chemistry

May 27, 2024

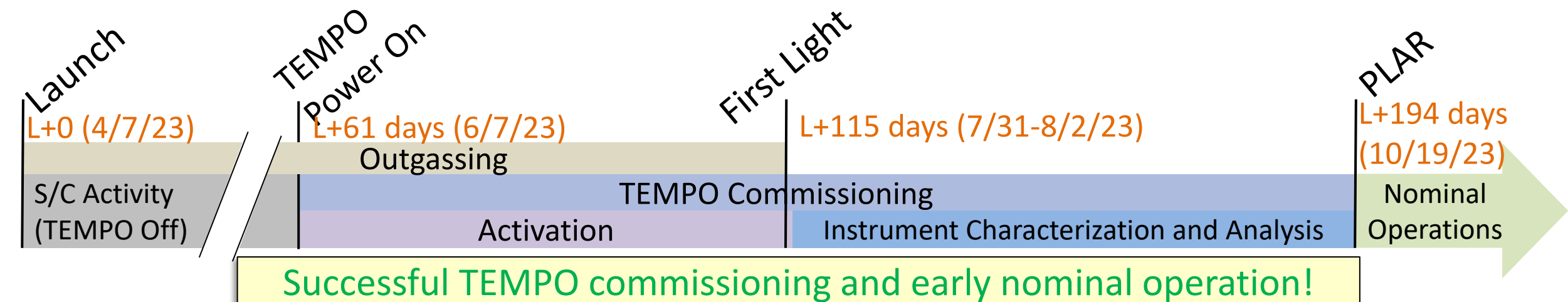




TEMPO Commissioning and Early Nominal Operation

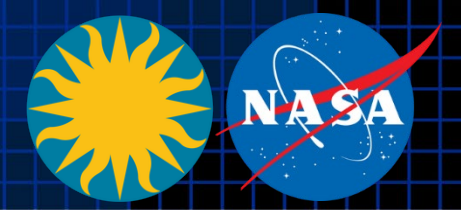


- **TEMPO commissioning: SAO + LaRC + Intelsat + Maxar + Ball + Carr Astronautics**
 - ✓ TEMPO power on 6/7, Dry out (6/9-7/9) and cool down (7/10-7/12)
 - ✓ First light (7/31-8/2): working/reference diffuser solar & Earth imaging
 - ✓ Instrument Characterization and Analysis (ICA) activities
 - ✓ Coordinate with AGES+ campaigns in Aug. and Coastal Texas Air Quality Field Campaign in Sep. (no Earth imaging for only 6 days, special observations over LA and Texas)
- **Nominal operation: after the Post Launch Acceptance Review (PLAR) on 10/18-19/2023**
 - ✓ Weekly commanding, no special observations before L2/3 public release
 - ✓ Optimize off-nominal twilight observations: city lights=>lighting types, Aurora, gas flaring, moonlight
 - ✓ Overall very smooth operation except for some data dropouts





Baseline Line Mission & Data Products Public Release Timeline



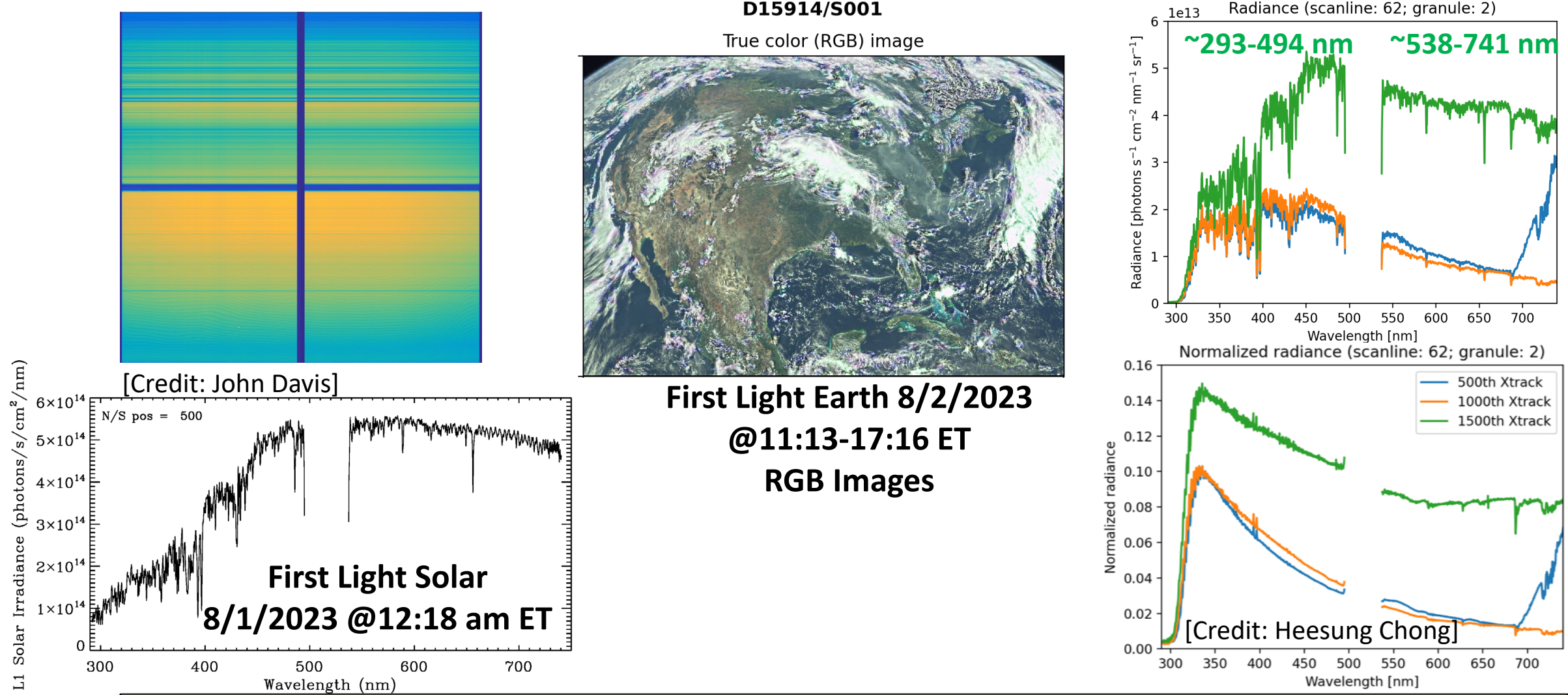
Data Product	Description	Time beyond On-Orbit Checkout (OOC) to deliver initial data	Maximum data latency after first release for $\geq 80\%$ of products
Level 0	Reconstructed, Unprocessed Instrument Data	2 months	Within 2 hours of receipt at SAO
Level 1b	Calibrated, Geolocated Radiances	4 months	Within 3 hours of Level 0 and ancillary data receipt at SAO
Level 2	Derived Geophysical Data Products	6 months	Within 24 hours of production of Level 1 at SAO
Level 3	Derived Gridded Geophysical Data Products	6 months	1 month after completion of data accumulation required for individual geophysical products

- **Baseline mission (Phase E, 20 months, 10/2023-6/2025), will be continued with NASA extension / senior review**
- **Data products sent to ASDC for archival & distribution before nominal operation**
- **Early access to TEMPO Science and Validation team members. Bi-weekly L2 Cal/Val meeting led by **Jim Szykman** & **Brad Pierce****
- **Mini release (Dec. 17-30, 8 days during Aug. commissioning) on Feb. 05, 2024**
- **Beta Level 1 public release: Feb. 27, 2024**
- **Level 2/3 public release: May 20, 2024**

We are nearly on track to release the data products to the public!

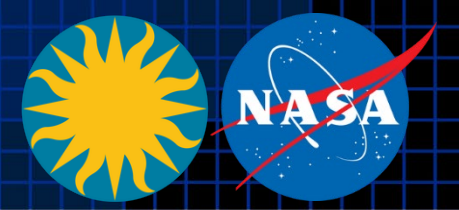


Imaging spectrometer measuring solar irradiance and solar backscattered Earth radiance





Baseline and Threshold Measurements Requirements



Species/Products	Required Precision	Temporal Revisit*
0-2 km O ₃ (Selected Scenes) Baseline only	10 ppbv	2 hour
Tropospheric O ₃	10 ppbv	1 hour
Total O ₃	3%	1 hour
Tropospheric NO ₂	1.0×10^{15} molecules cm ⁻²	1 hour
Tropospheric H ₂ CO	1.0×10^{16} molecules cm ⁻²	3 hour

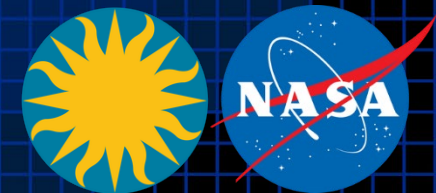
- * # of hourly measurements to be averaged to achieve required precision
- Mission duration: 20 months for baseline, 12 months for threshold
- Spatial resolution: < 60 km² for baseline (4 native pixels coadded), < 300 km² for threshold
- AOD, SO₂, and CHOCHO removed at KDP-C.

Reduced list of baseline data products due to cost cap!



TEMPO Data Products

Baseline + SNWG TEMPO NRT



Level	Product	Algorithm	Major Outputs	A Priori (L2)	Res km ² *	Freq/Size	Val. Status (5/20/2024)
L0	Digital counts	Raw to L0	Reconstructed/reformatted DN		2.0 x 4.75	Daily/hourly	
L1	Irradiance ^{NRT}	SAO L0-1	Calibrated & quality flags			weekly	Beta
	Radiance ^{NRT}	SAO L0-1	Geolocated, calibrated, viewing, geolocation & quality flags		2.0 x 4.75	Hourly, granule	Beta
	City lights	SAO L0-1	Geolocated & calibrated		2.0 x 4.75	Variable, granule	Beta
L2	Cloud ^{NRT}	OMI O ₂ -O ₂	Cloud fraction, cloud pressure	GEOS-CF	2.0 x 4.75	Hourly, granule	Beta
	O ₃ profile	SAO O ₃ profile	O ₃ profile, total/strat/trop/0-2 km O ₃ column, errors, a priori, AKs	Climatology+ GEOS-CF	>= 8.0 x 4.75**	Hourly, granule	Unvalidated
	Total O ₃	TOMS V8.5	Total O ₃ , AI, cloud fraction	Climatology	2.0 x 4.75	Hourly, granule	Beta
	NO ₂ ^{NRT}	SAO trace gas, BU strat./trop. sep.	SCD, strat./trop. VCD, error, shape factor, scattering weights	GEOS-CF	2.0 x 4.75	Hourly, granule	Beta
	HCHO ^{NRT}	SAO trace gas	SCD, VCD, error, shape factor, scattering weights	GEOS-CF	2.0 x 4.75	Hourly, granule	Beta
L3	Gridded L2	SAO L2-3	Same as L2		2 x 2	Hourly, scan	

* Spatial resolution at center of FOR. ** Might be at 8 x 9.5 km²

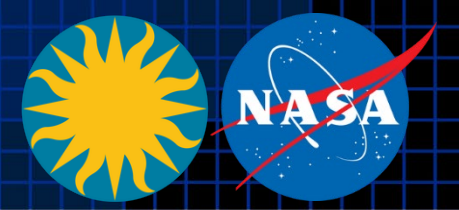
Research **aerosols, SO₂, ocean color** products

Satellite Needs Working Group (SNWG) funded TEMPO NRT products (L2 products < 3 hours from observation time):

3/26/2024-3/25/2026, NOAA GeoXO team to produce TEMPO/GOES-R NRT aerosol products



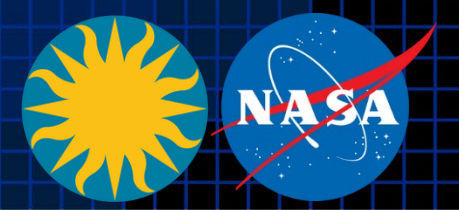
Algorithm/Data Products Development Timeline



- **First Light NO₂ Images Release (8/24):** updates to pre-launch (SDPC v4.0) (offline/development):
 - ✓ Use initial wavelength grid for radiance from calibrated first light working solar irradiance
 - ✓ No straylight correction and polarization correction
 - ✓ Optimized Image Navigation and Registration (INR) for first light
 - ✓ Optimization to clouds & NO₂ algorithms
- **First official SDPC update: SDPC v4.1 (V1 data products)** approved on 10/16, operational on 10/17, L0-1b, cloud, NO₂, HCHO, total O₃ produced and sent to ASDC
 - ✓ INR: working well meeting science requirements.
 - ✓ L0-1b: gain/non-linearity, bad pixel map, improved saturation flagging, Octant phase (odd/even)
 - ✓ Further optimization in cloud and NO₂
 - ✓ Major changes to HCHO: radiance reference, and background/reference correction
 - ✓ O₃ profile not ready due to absolute radiometric calibration
- **SDPC v4.2 (V1):** approved on 11/17, operational on 11/18
 - ✓ INR: remove UV/Visible biases, accurate at subpixel level, tested to work for special observation
 - ✓ Data processing pipeline: more robust, automatically recover from INR crash, other minor updates
 - ✓ Used to reprocess TEMPO commissioning observations



Algorithm/Data Products Development Timeline

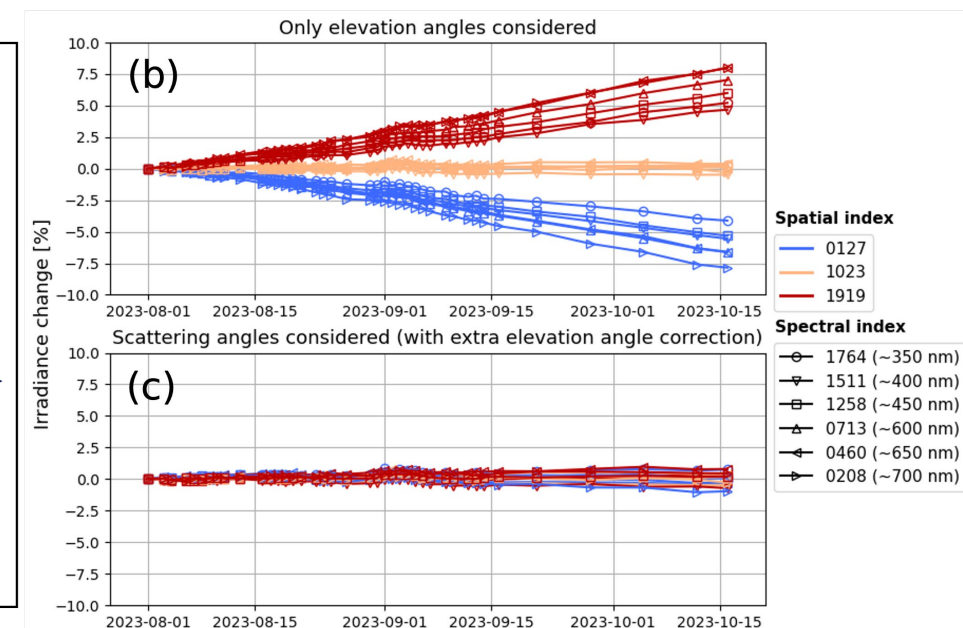
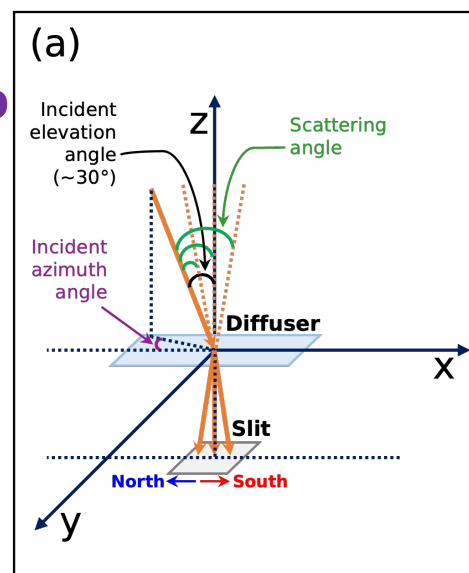


➤ SDPC v4.3 (V2) & Level 1 release: approved on 2/23/2024, operational 2/26/2024

✓ Level 1 Beta Public Release:

- ❖ Scattering angle dependent BTDF correction, removing time- and across-track dependent biases
- ❖ Improved CCD image processing steps (electronic offset correction, smear correction, dark current correction after accounting for temperature dependence)
- ❖ Improved solar wavelength calibration, use latest solar irradiance wavelength for radiance

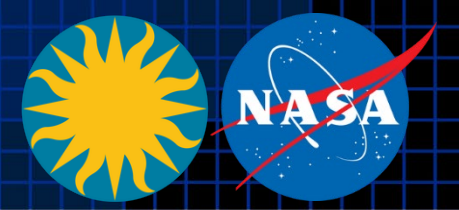
- ✓ Critical updates to NO_2 , HCHO, and cloud algorithms: GLER interpolation issues, snow/ice, missing data due to cloud radiance wavelength calibration failure, NO_2 tropopause layer selection bug, temperature correction in total NO_2 AMF
- ✓ Change L3 resolution from $0.05^\circ \times 0.05^\circ$ to $0.02^\circ \times 0.02^\circ$



[Credit: David E. Flittner]



Algorithm/Data Products Development Timeline

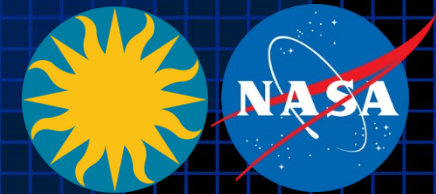


- **SDPC v4.4 (V3) & Level 2-3 release: May 20, 2024**
 - ✓ **Improved Level 1 & new Level 1 city lights**
 - ❖ Add nominal geolocations for city lights & Improve the robustness for INR
 - ❖ Improve FPA temperature sampling and temperature-dependent dark current correction
 - ❖ Add straylight correction (1-D PSF)
 - ❖ Add radiance wavelength calibration
 - ✓ **Improved Level 2 & 3 and likely ozone profile (UV only) product for public release**
 - ❖ Update GLER (v6.0->v6.1, snow free + 100% snow, quality flag 2-> 5, fill in gaps via interpolation)
 - ❖ Perform retrievals up to SZA 90
 - ❖ Update main data quality flag (AMF > 6 as suspect), Revisit convergence flag & AMF diagnostic flag
 - ❖ Add temperature profile to output (for AMF)
 - ❖ Cloud: SCD fitting optimization, SCD T correction, ECF/OCP iteration, wavelength shifts to ECF
 - ❖ **Ozone profile: Update the use of GEOS-CF meteorology and ozone profile + Derive soft calibration**
- **After the May 2024 L2/3 public release --- end of baseline mission:**
 - ✓ **Reprocessing for all data products (except for ozone profile product)**
 - ✓ **Updates to science algorithms & calibrations as needed based on validations and feedback**
 - ✓ **Update O₃ profile retrieval with UV only**
 - ✓ **Release UV/Visible to improve retrieval sensitivity to 0-2 km O₃**

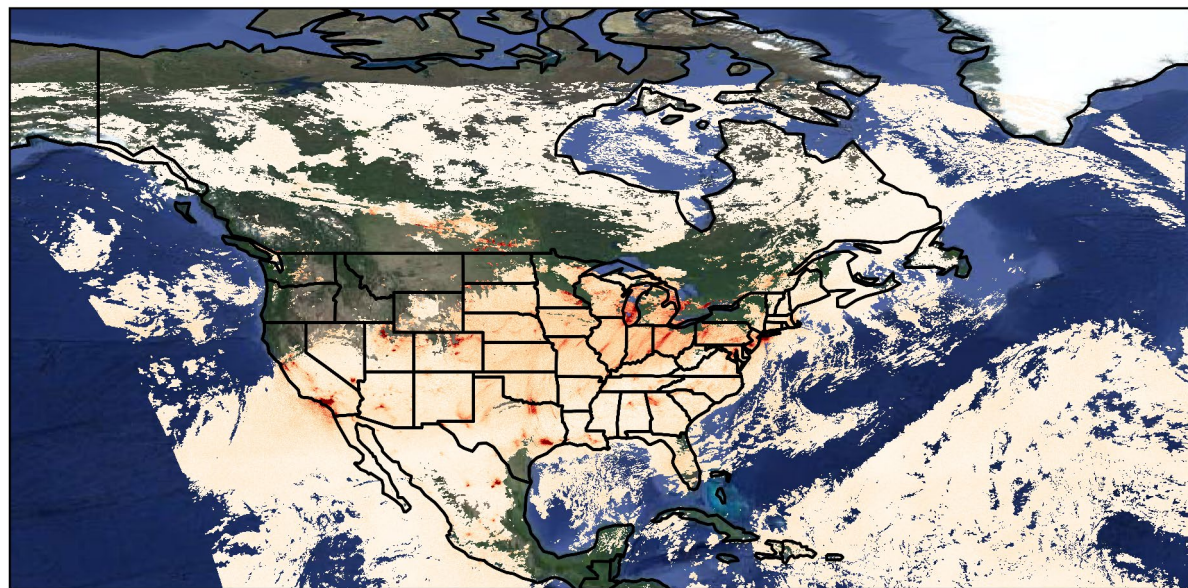
Power/cooling issues at our data center



TROPOMI and TEMPO NO₂



TROPOMI tropospheric NO₂ column
02 November 2023

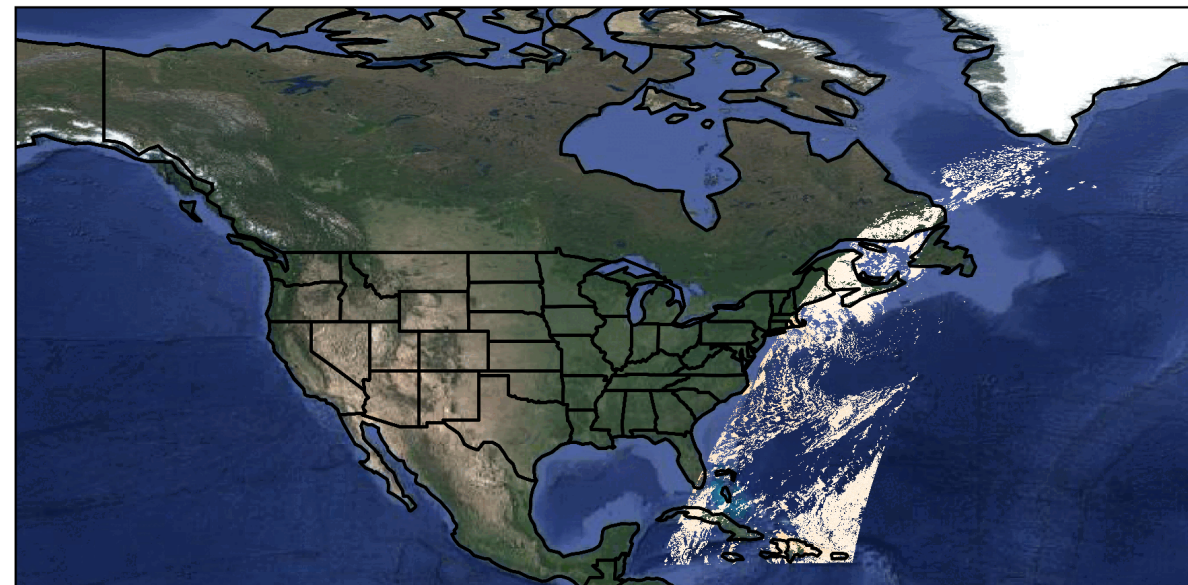


Basemap Google (c)

mol/m²



TEMPO tropospheric NO₂ column
02 November 2023
Scan 001 (11:41:46 UTC)



Basemap Google (c)

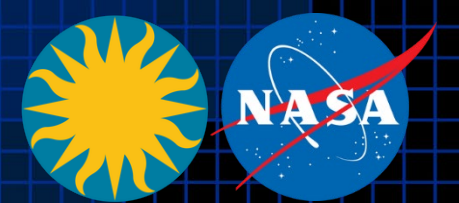
molecules/cm²



[Credit: Caroline Nowlan]

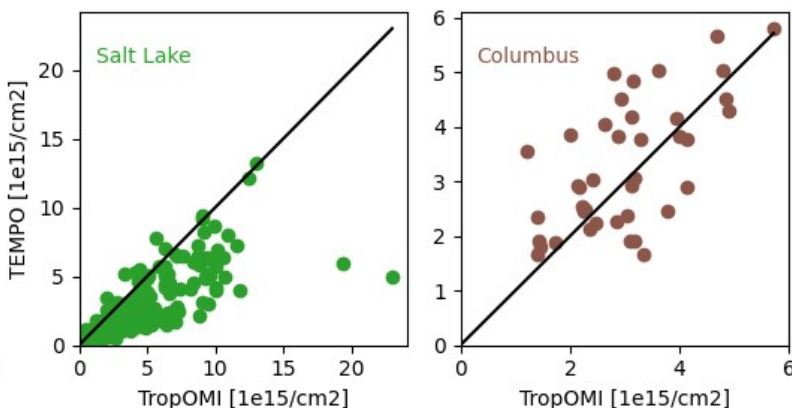
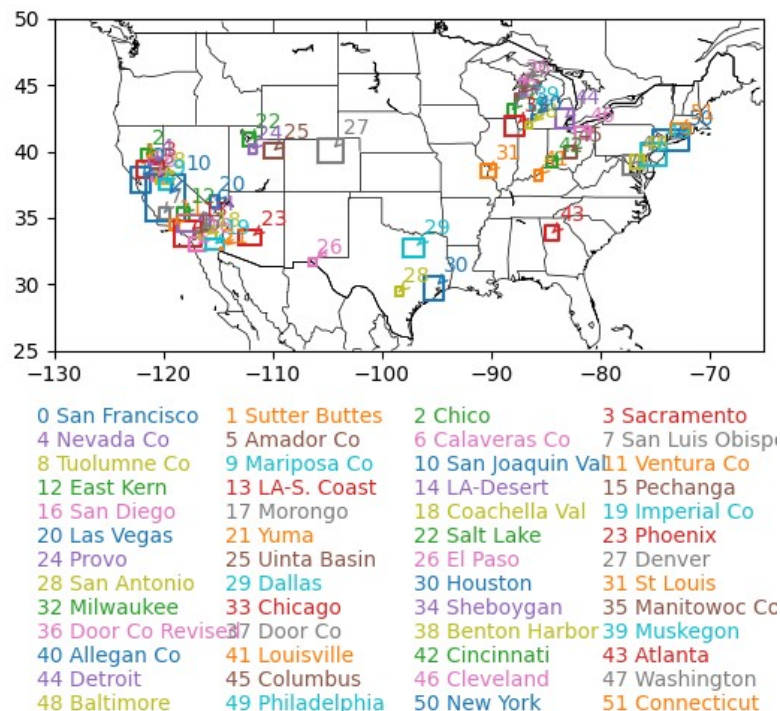
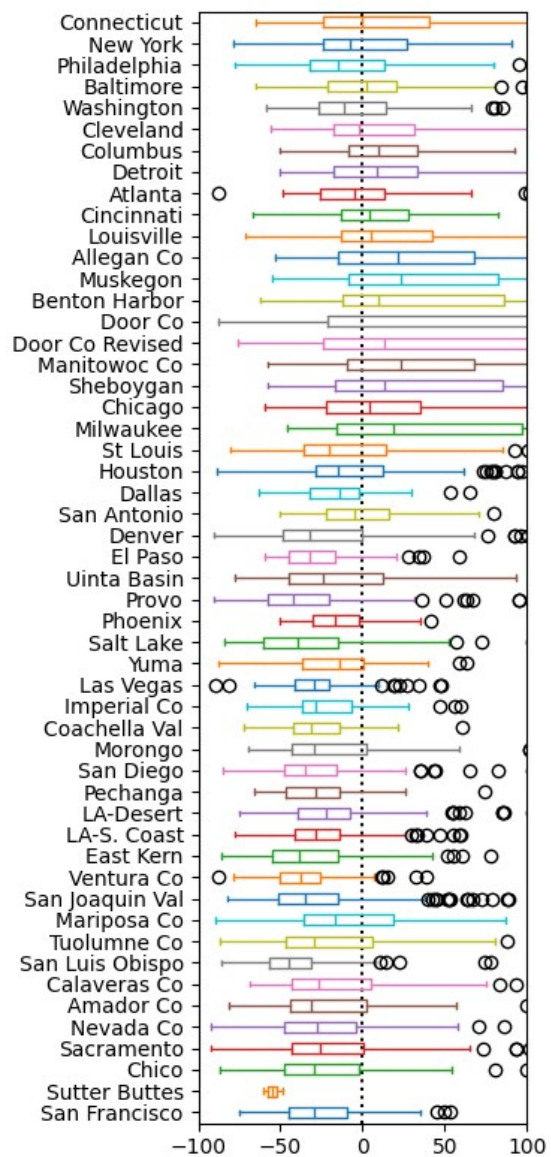


TROPOMI NO₂ Comparisons



Courtesy of Barron Henderson, EPA

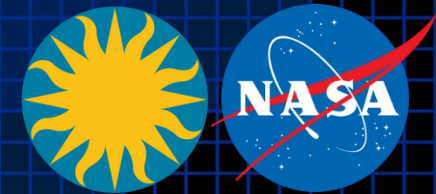
PRELIMINARY!!



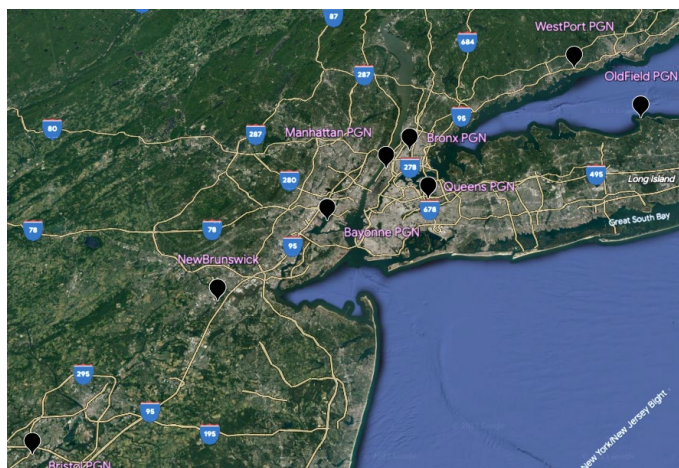
- Overall, TEMPO tropospheric NO₂ agrees well with TROPOMI
- Biases between products can be due to differences in AMF inputs
- Larger negative TEMPO bias in western U.S.?



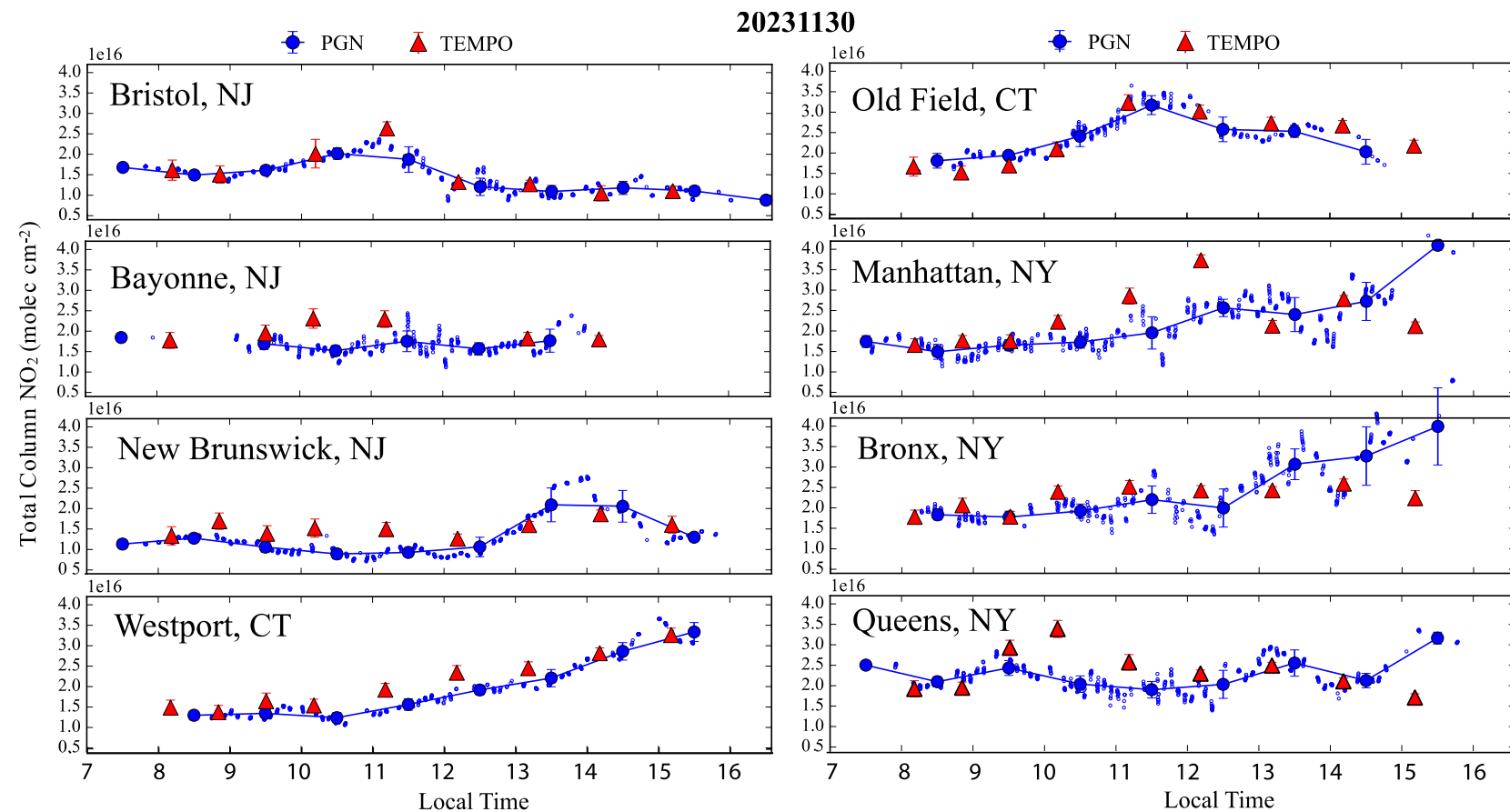
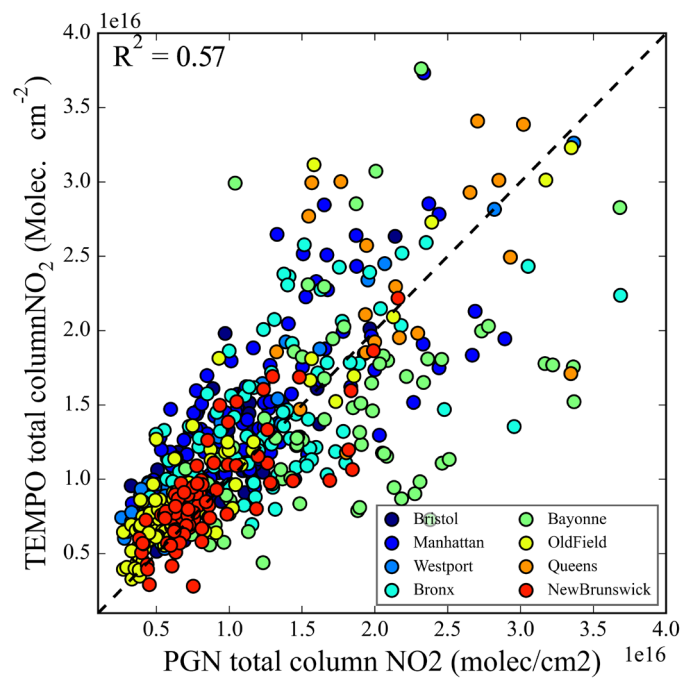
Pandora NO2 Comparisons



Courtesy of Prajwal Rawat (NASA LaRC), Katherine Travis (NASA LaRC), James Szykman (EPA)



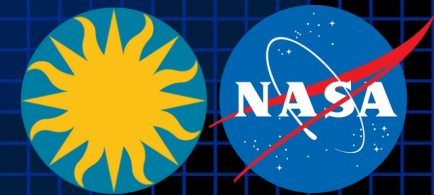
November 23-Jan 20



PRELIMINARY!!



TEMPO and TROPOM HCHO (29-30 August 2023)

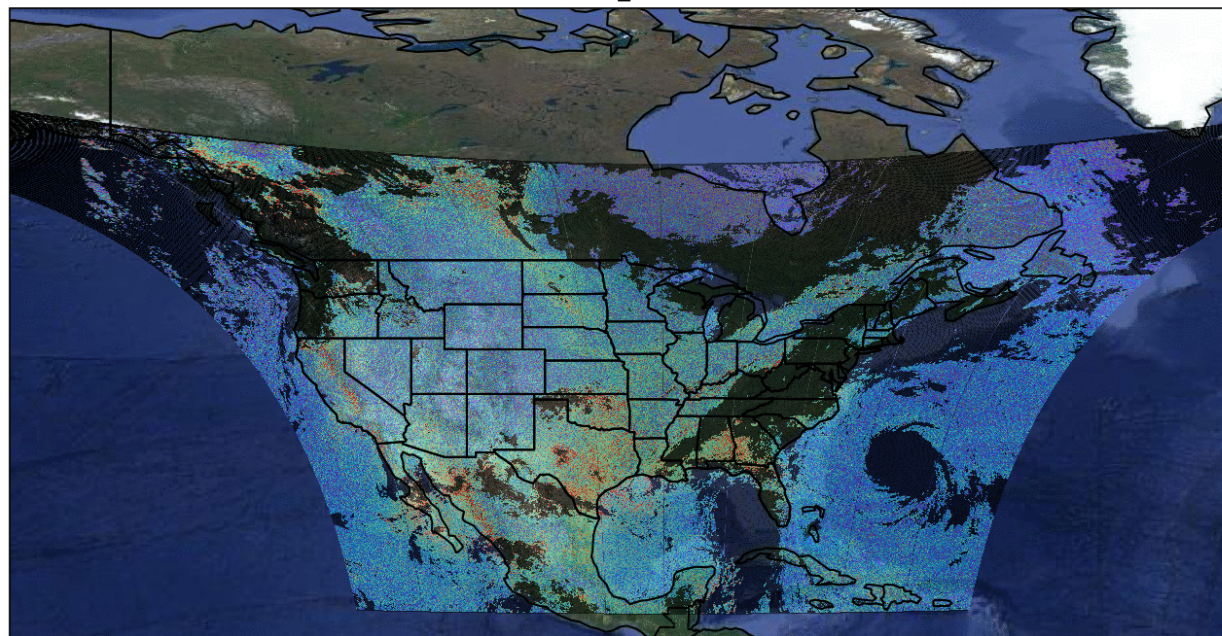


Google Engine S5P HCHO 0829

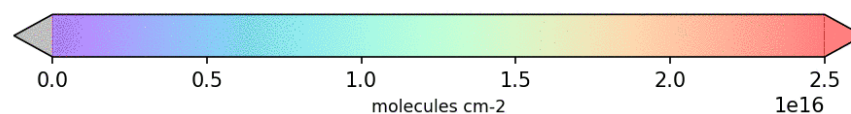
Google Engine S5P HCHO 0830

D15941_S007: 2023-08-29 14:15:28 to 2023-08-29 15:11:25

vertical_column



TEMPO HCHO 0829-0830 (scans close to S5P overpass)

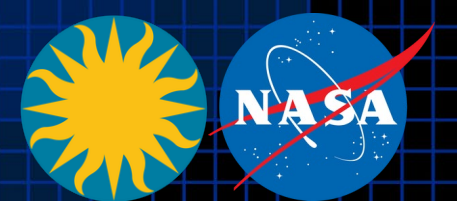


- TEMPO vs TROPOMI shows spatial agreement in HCHO columns. TEMPO shows small noise and almost no striping. Systematic biases are expected associated with AMF, radiance reference and background corrections.

[Credit: Gonzalo Gonzalez Abad]

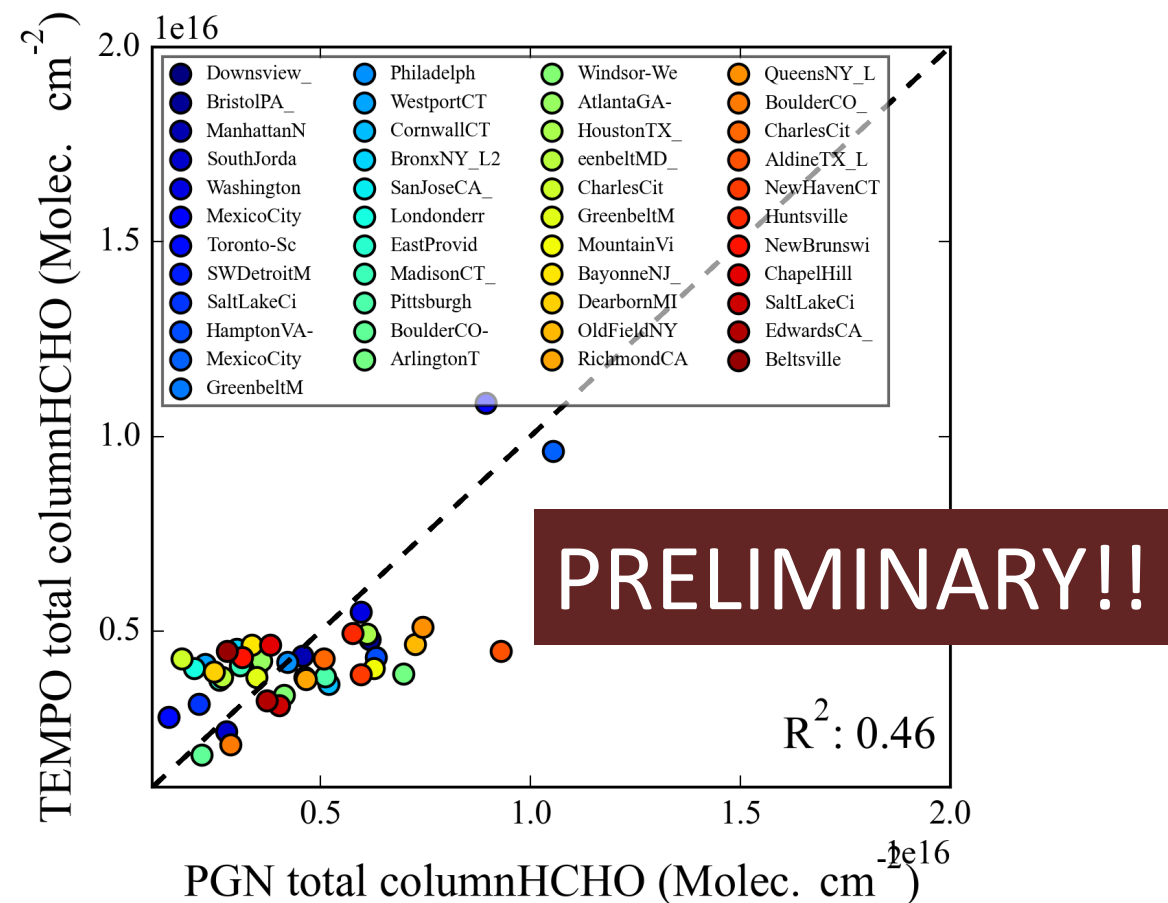
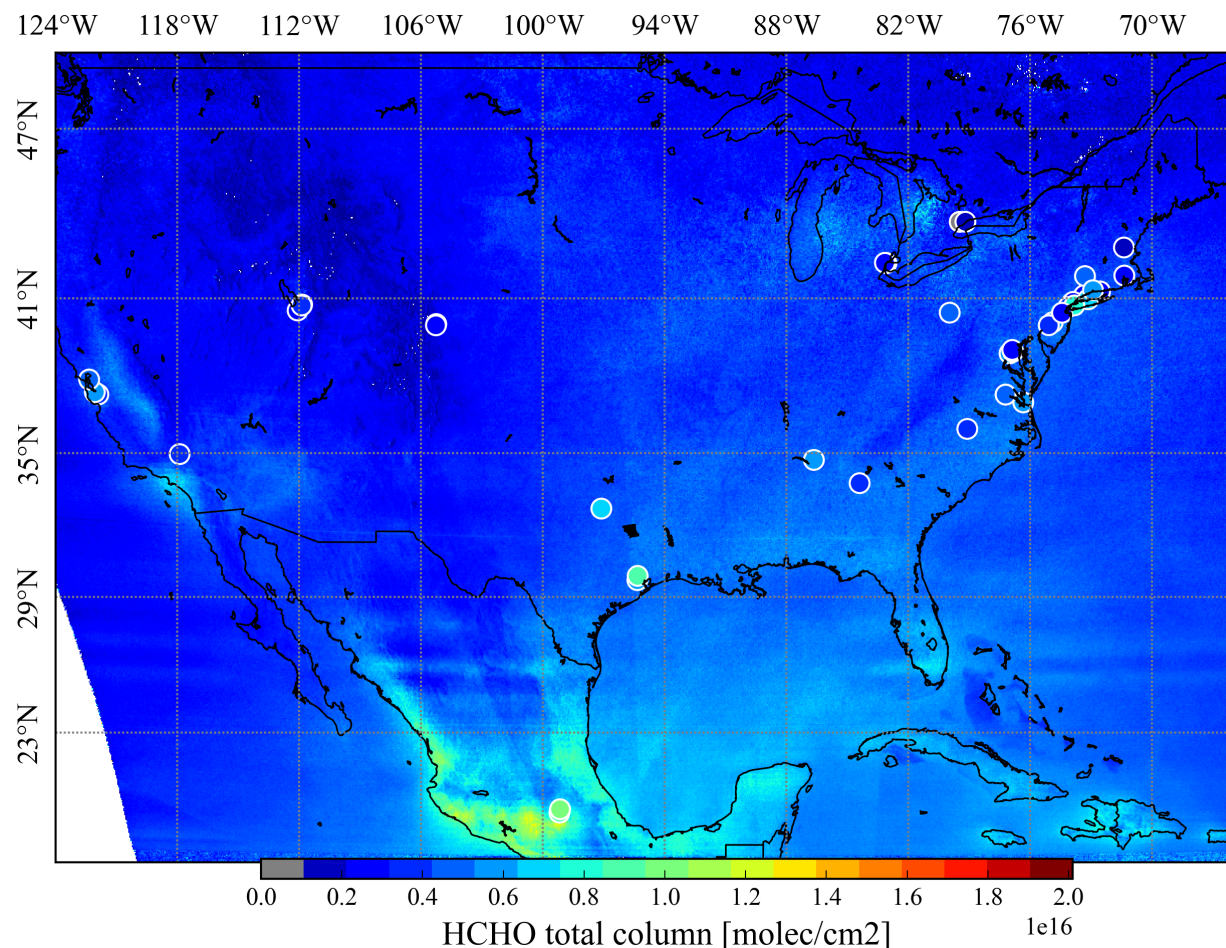


Pandora HCHO Comparisons



November 23-Jan 20

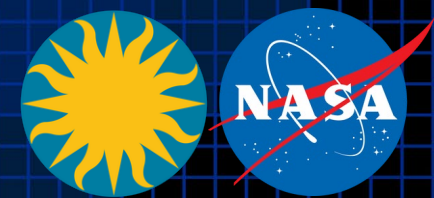
Courtesy of Prajwal Rawat (NASA LaRC), Katherine Travis (NASA LaRC), James Szykman (EPA)



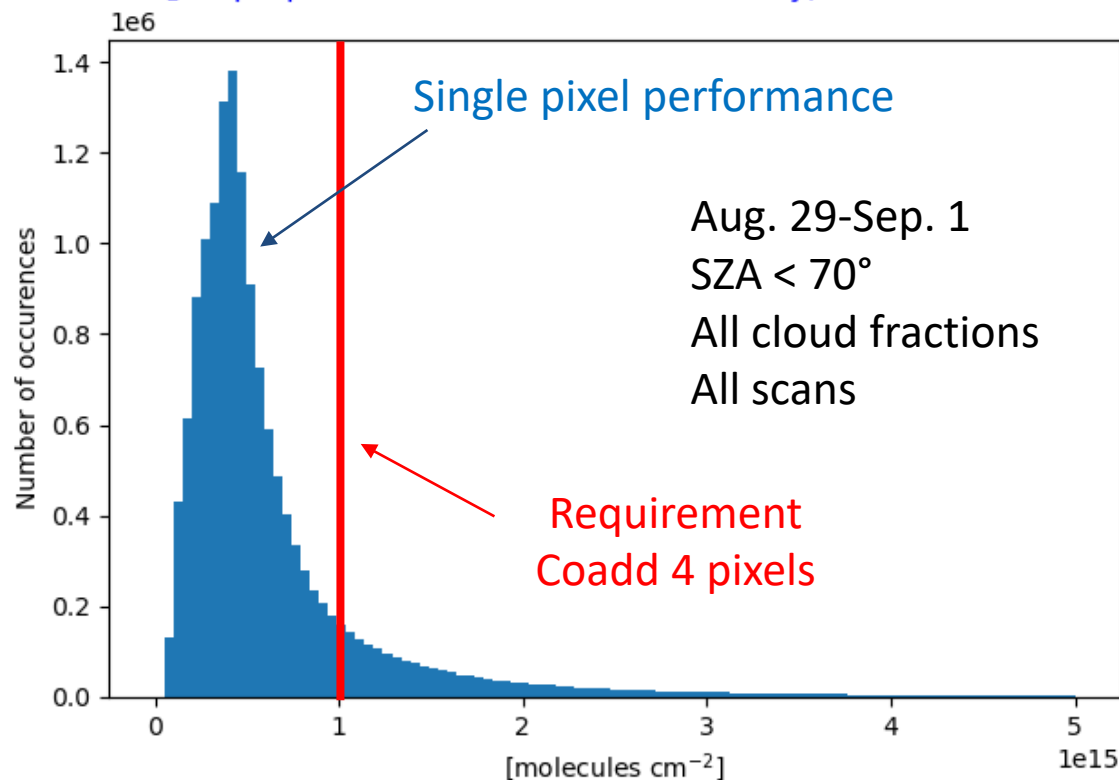
- HCHO hotspots are captured well by both the measurements, irrespective of Pandora locations.
- A moderate spatial correlation is observed between Pandora direct Sun HCHO and TEMPO HCHO column with larger dynamical range in the Pandora observations.



NO₂ Tropospheric Column & HCHO Column Uncertainties

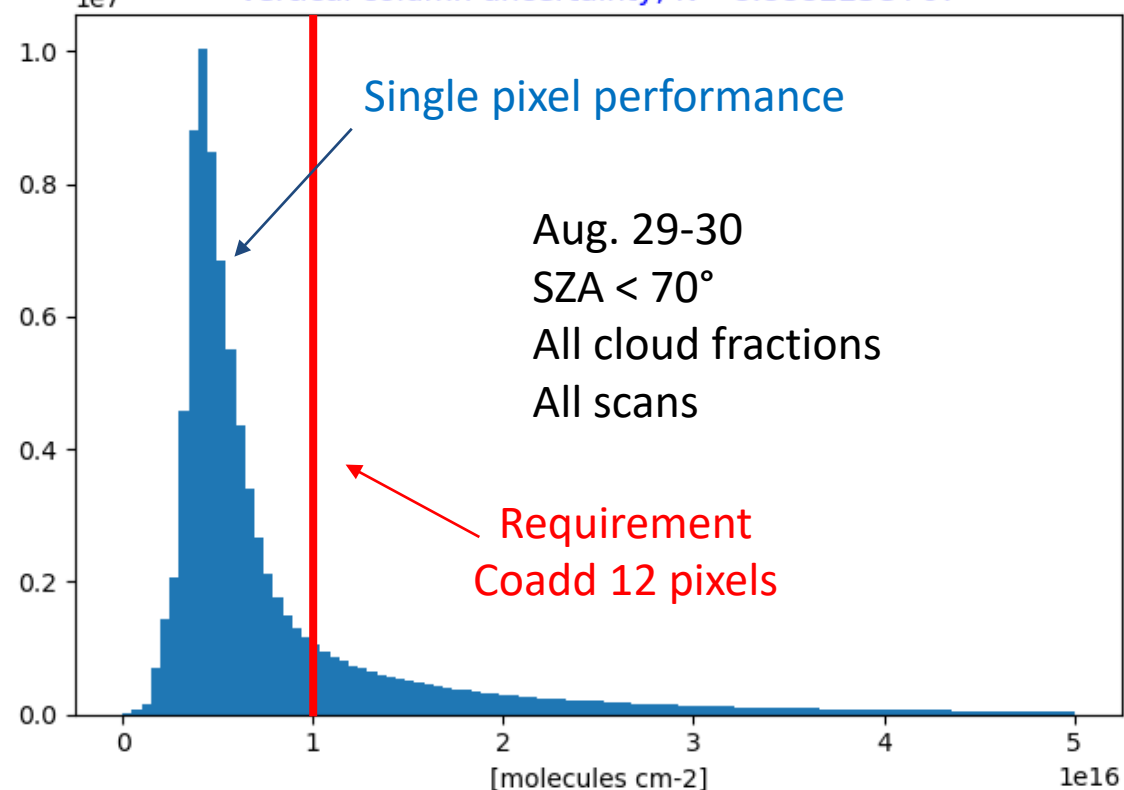


NO₂ tropospheric vertical column uncertainty; N ~1.454321e+07



- NO₂ Median uncertainty = 0.46×10^{15} molecules/cm² (SZA < 70°, all clouds)

Vertical column uncertainty; N ~8.888223e+07

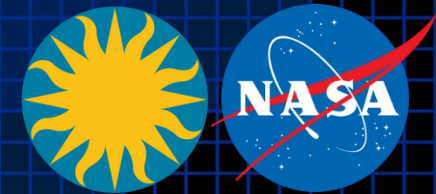


- HCHO Median uncertainty = 5.5×10^{15} molecules/cm² (SZA < 70°, all clouds)

TEMPO NO₂ & HCHO meets requirement for >90% of cloud-free scenes with **no pixel coadding!**

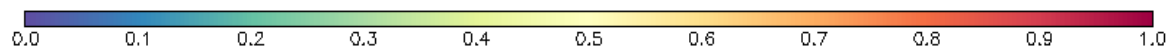
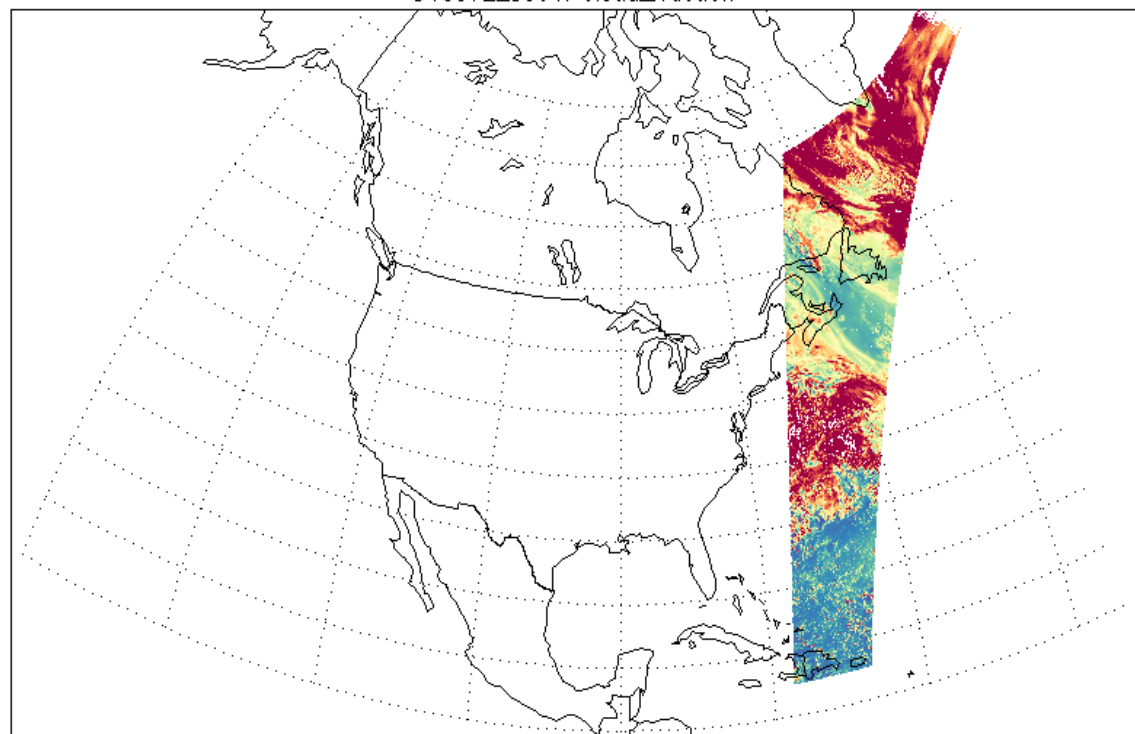


Cloud Products (29 September 2023)



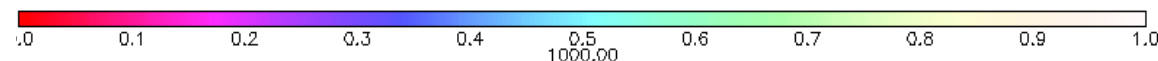
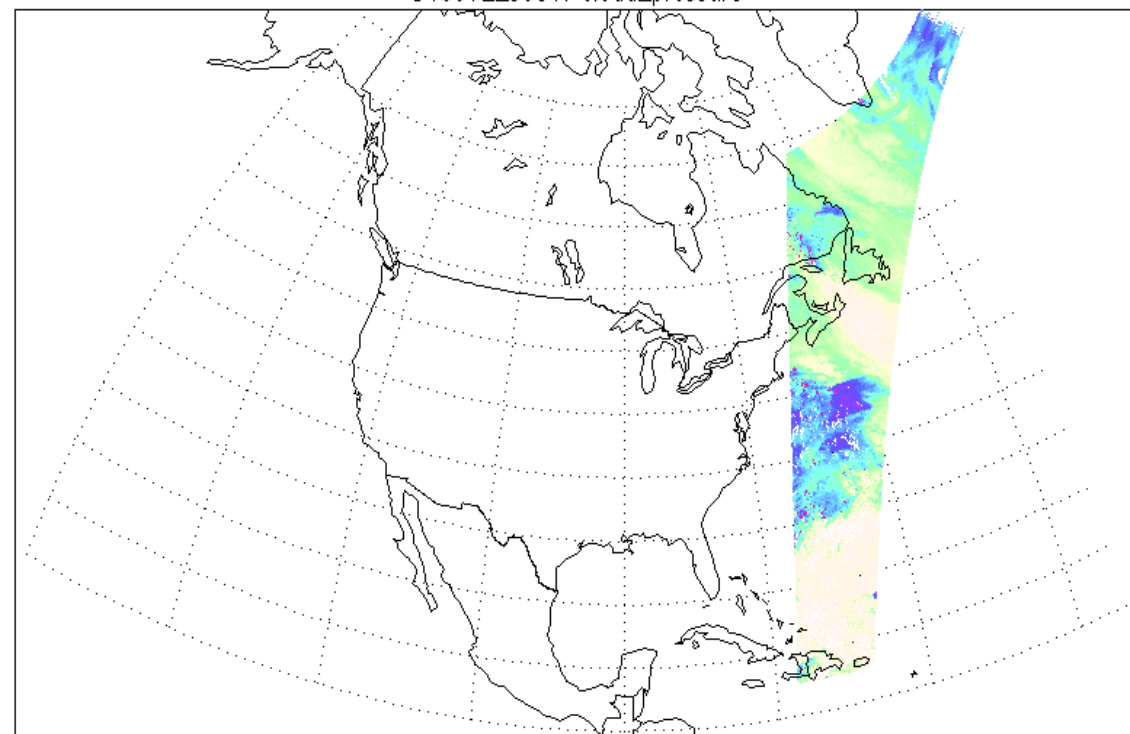
Cloud fraction

D15972_S001: cloud_fraction



Cloud pressure

D15972_S001: cloud_pressure

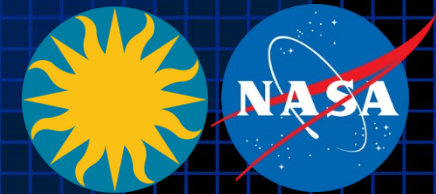


➤ Saturation causes no retrieval under very cloudy conditions.

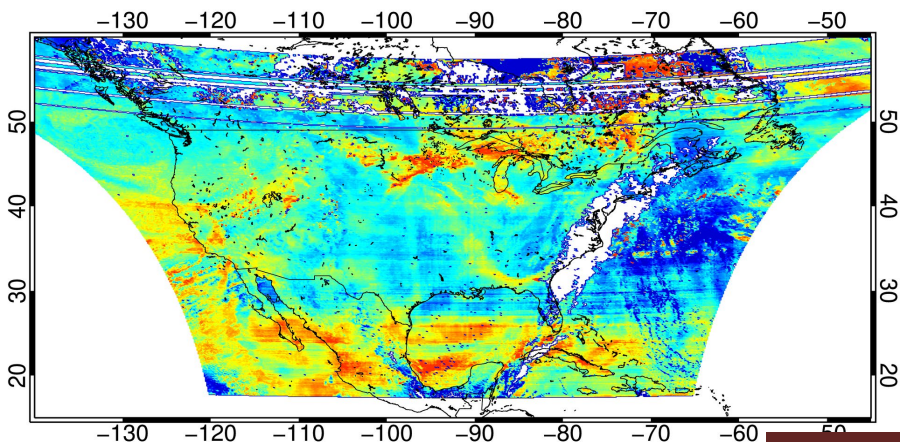
[Credit: Huiqun Wang]



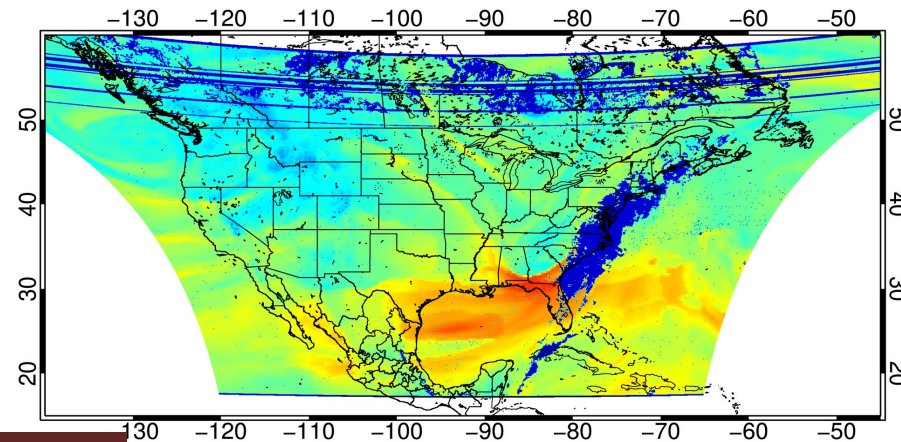
TEMPO O3PROF (3/28/2024 Scan 008)



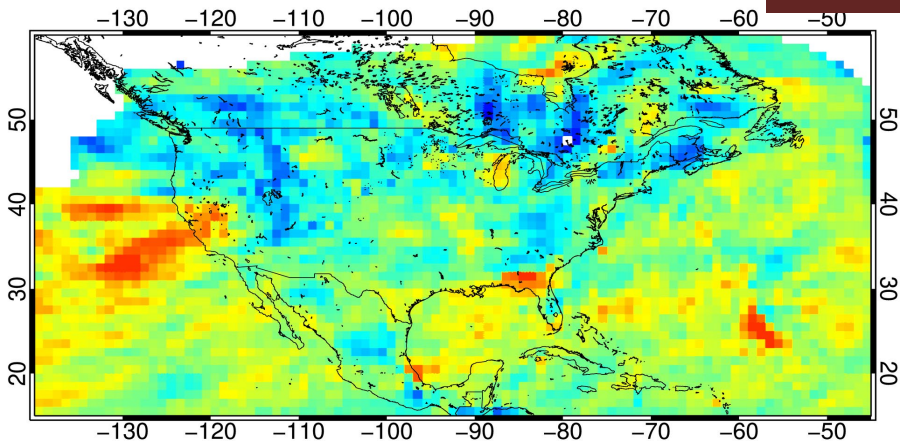
Tropospheric O3 from TEMPO O3PROF



Tropospheric O3 from GEOS-CF

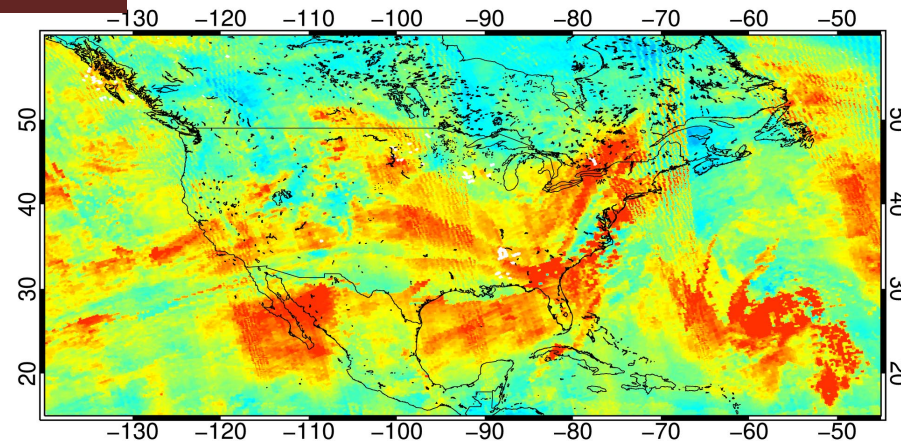


Tropospheric O3 from EPIC

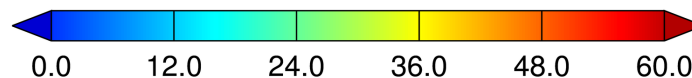


PRELIMINARY!

Tropospheric O3 from TROPOMI



Dobson Unit



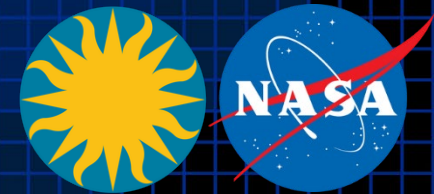
[Credit: Jerry Ziemke]

Note different tropopause pressure from EPIC/TROPOMI!

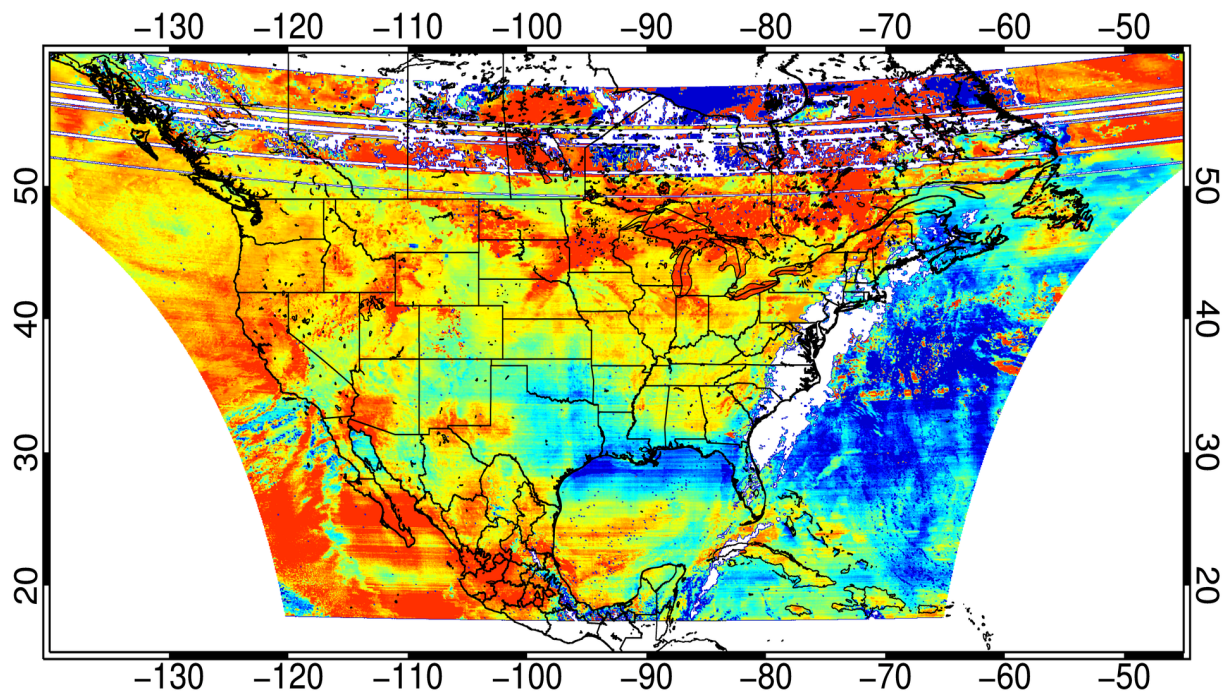
[Credit: Junsung Park]



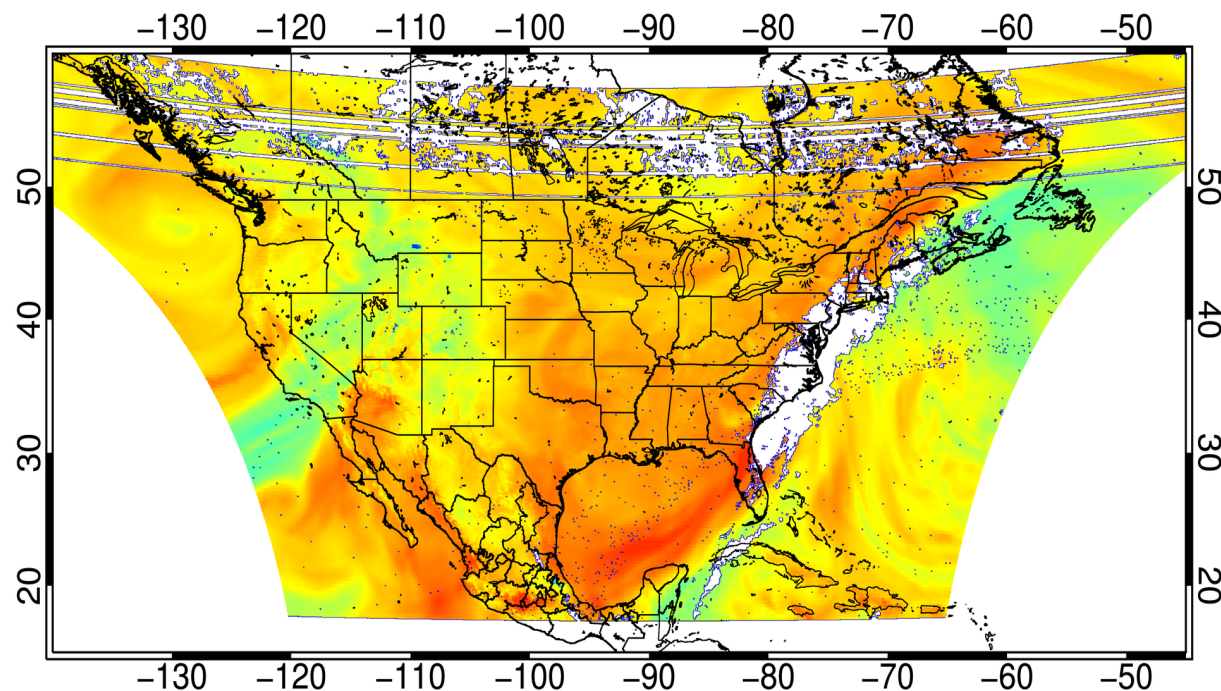
TEMPO O3PROF (3/28/2024 Scan 008)



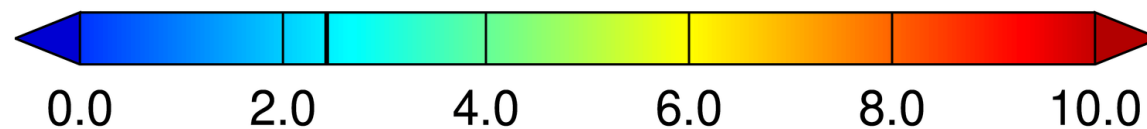
Surface to 2 km O3 from TEMPO O3PROF



Surface to 2 km O3 from GEOS-CF



[Credit: Junsung Park]

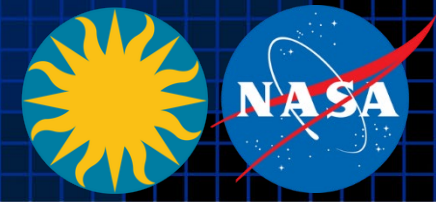


Dobson Unit

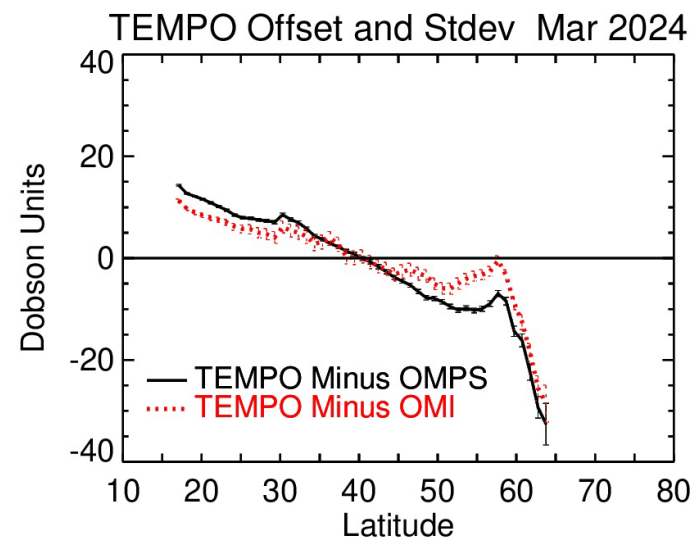
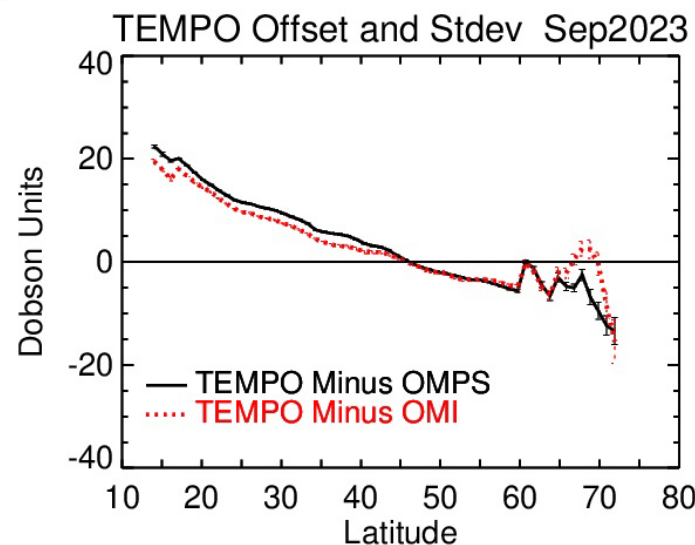
PRELIMINARY!



TEMPO Total Ozone (V2): Comparison with OMPS and OMI



*Credit: Jerry
Ziemke & Stacey
Frith, NASA GSFC*

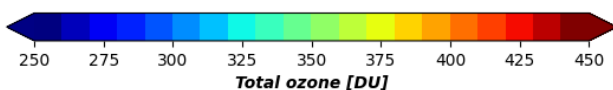
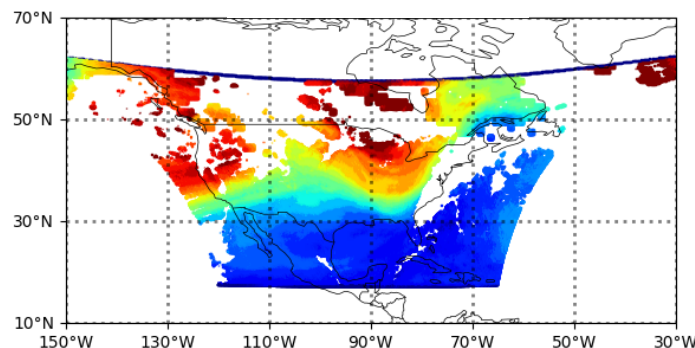


OMPS and OMI
within ± 3 hr overpass
with TEMPO with all
data binned to $1^\circ \times 1^\circ$
daily averages

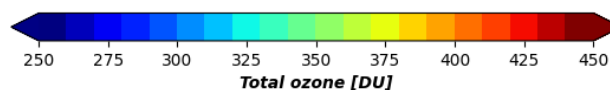
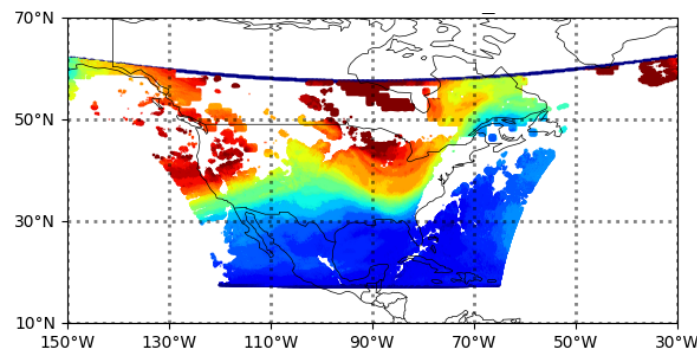
20240328, S008

CF < 0.3

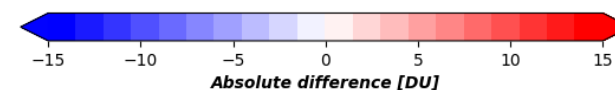
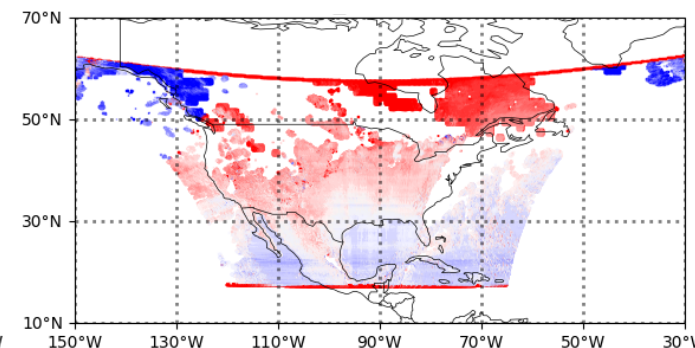
V2



V3

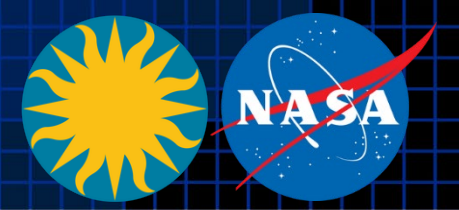


V3 - V2





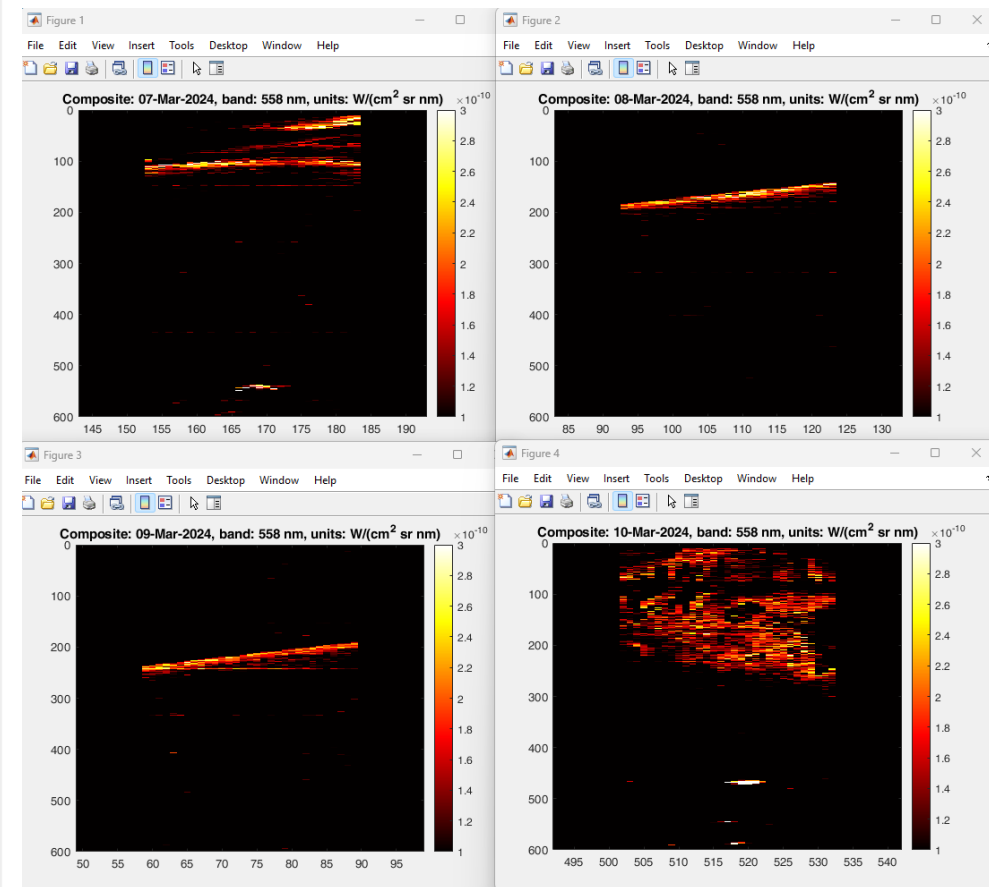
City Lights & Aurora



Clearest-Sky Composite 1–12 February 2024



Oxygen at 558 nm

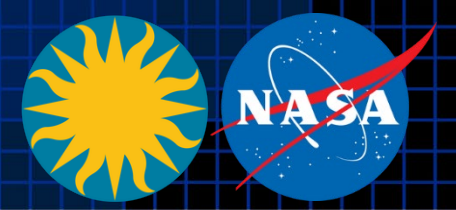


Radiance derivation → Post-processing (de-speckling, de-streaking, etc.) → Composite

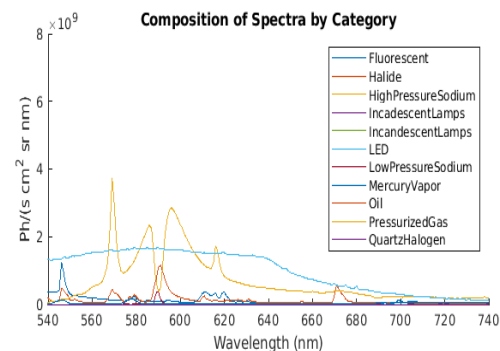
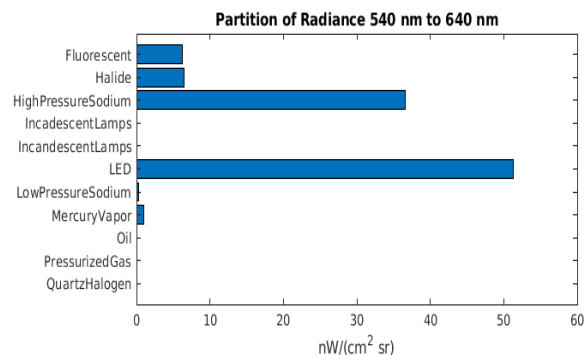
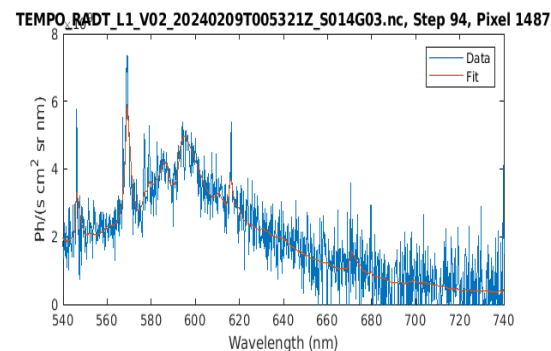
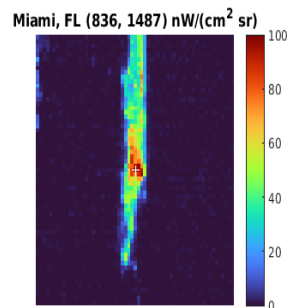
[Credit: Jim Carr]



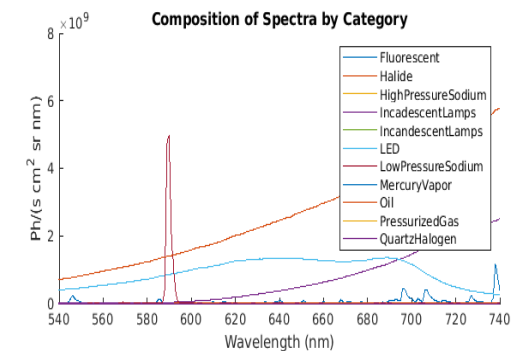
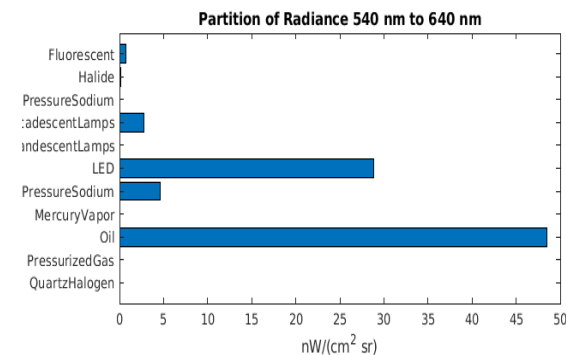
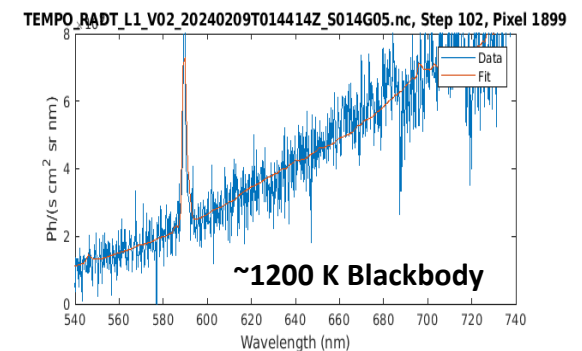
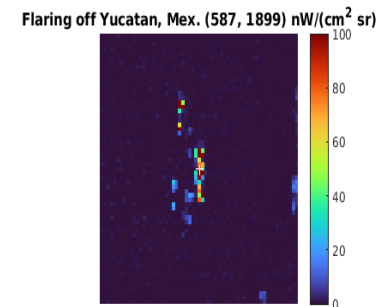
City Lights Spectral Classification



Miami, FL

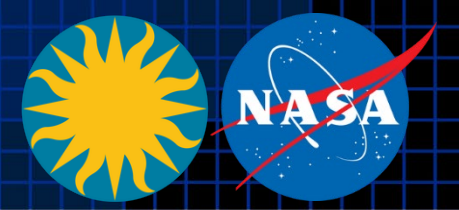


Offshore Flaring





Summary

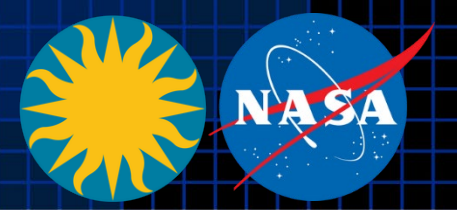


- TEMPO commissioning and nominal operation have gone on very well
- TEMPO is providing revolutionary hourly daytime atmospheric pollution measurements at high spatial resolution over North America
- Most data products (L1b, cloud, NO₂, HCHO, total O₃) are in good quality at this early stage, showing that the TEMPO instrument and science algorithms are working very well.
- We are on track to release the L2/3 data products to the public (likely including the UV only ozone profile product)

On track to release TEMPO data products that are acceptable to enable meeting baseline science requirements!

Acknowledgements: Funding from
NASA (Contract No. NNL13AA09C)

Thank you!



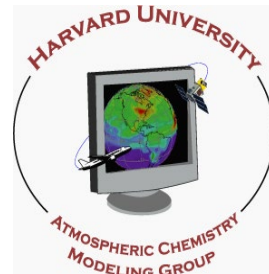
CENTER FOR
ASTROPHYSICS
HARVARD & SMITHSONIAN



MAXAR



LAH
THE UNIVERSITY OF
ALABAMA IN HUNTSVILLE



CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS


THE UNIVERSITY
OF IOWA

YORK
UNIVERSITÉ
UNIVERSITY



 **INECC**
INSTITUTO NACIONAL
DE ECOLOGÍA
Y CAMBIO CLIMÁTICO



FINNISH METEOROLOGICAL
INSTITUTE



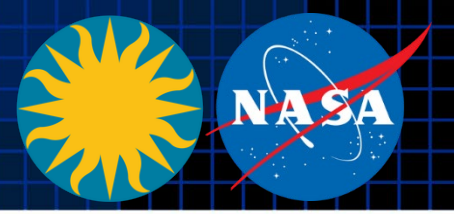
NCAR



Environment and
Climate Change Canada

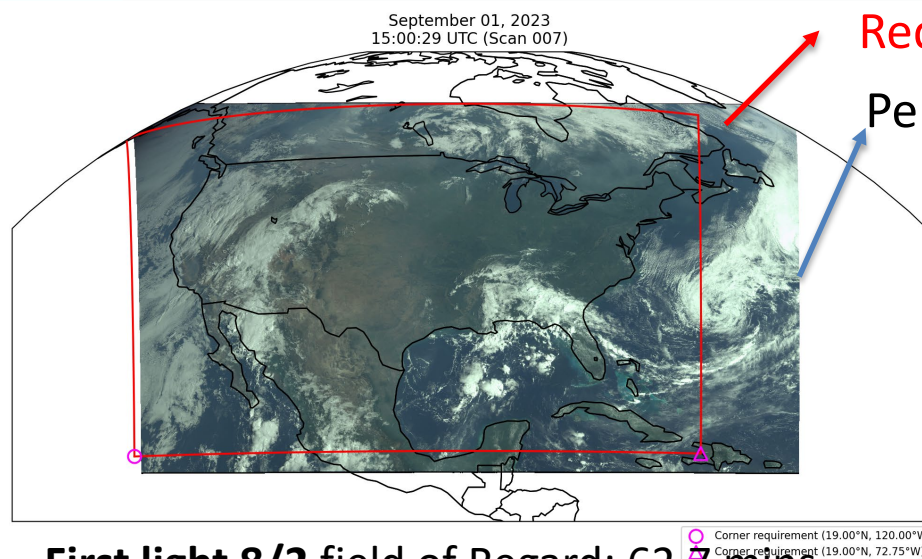
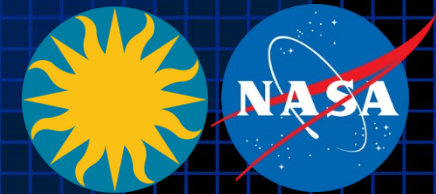
Environnement et
Changement climatique Canada





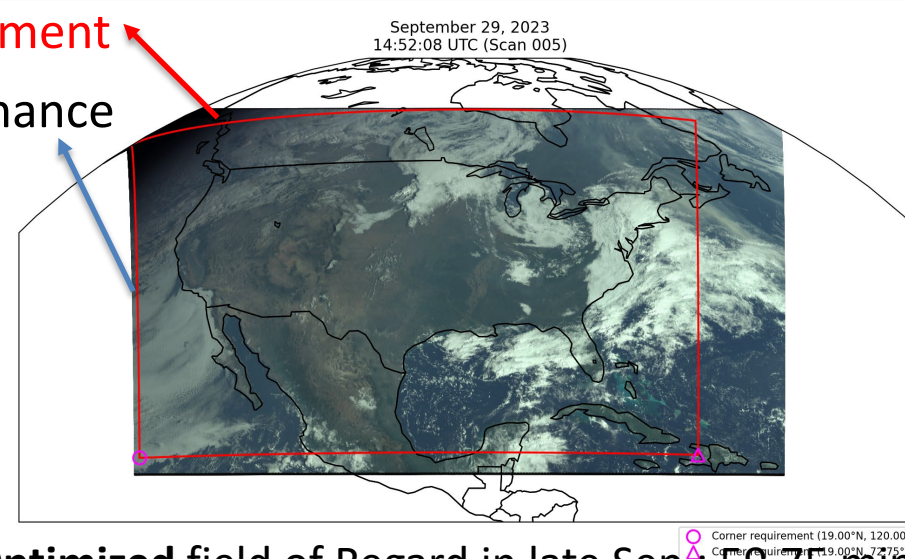


Field of Regard



First light 8/2 field of Regard: 62.7 mins

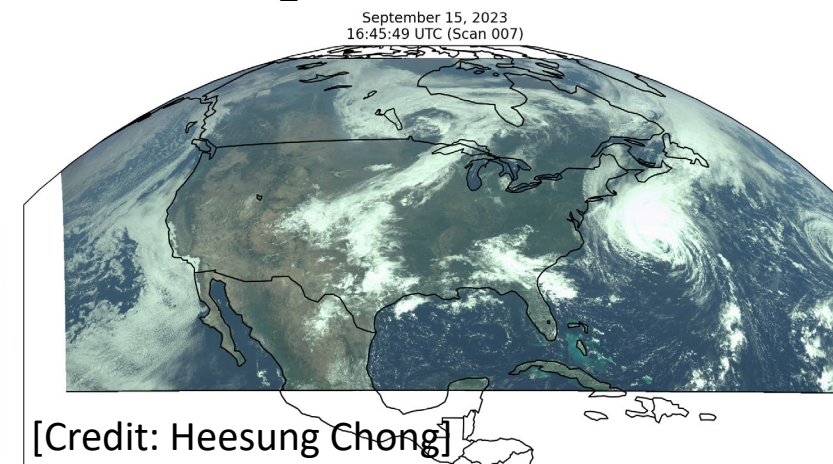
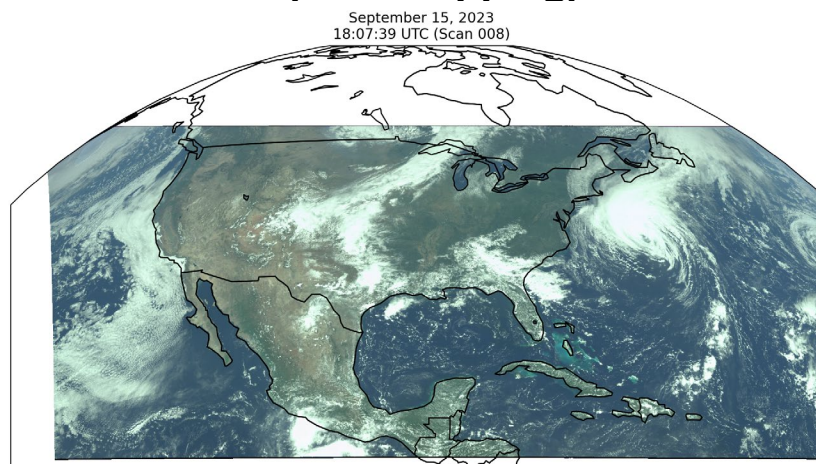
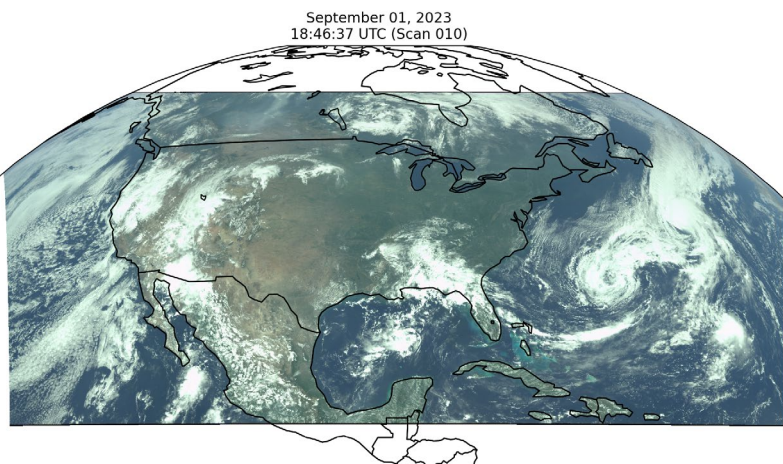
(100 ms integration time, 26 coadds, 61.5 μ rad)



Optimized field of Regard in late Sep.: 59.75 mins

(100 ms integration time, 26 coadds, 64 μ rad)

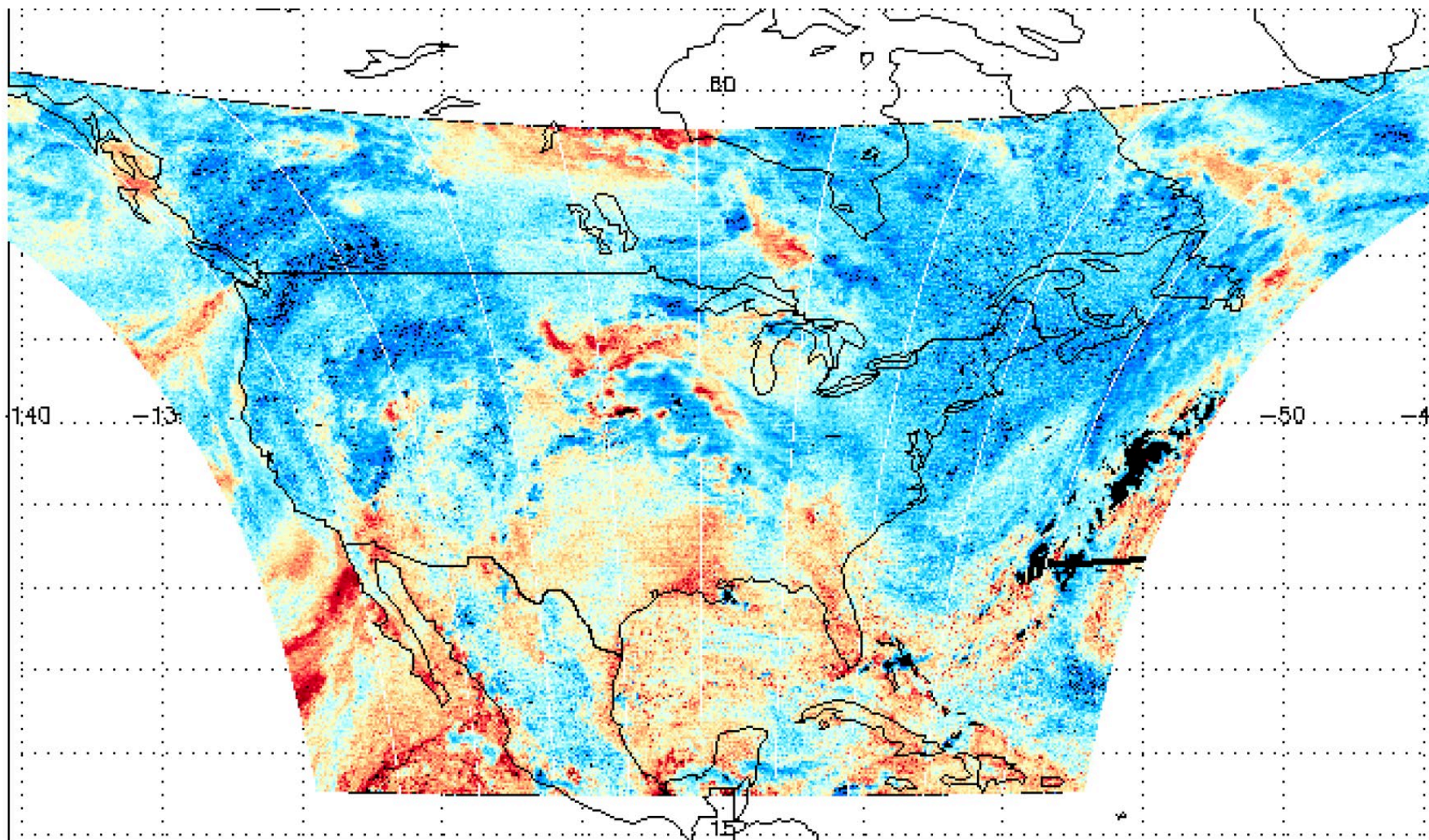
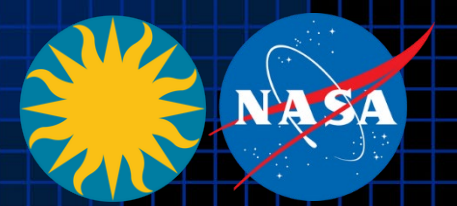
Fields of regard characterization (FOR mapping) with different N-S SMA angles



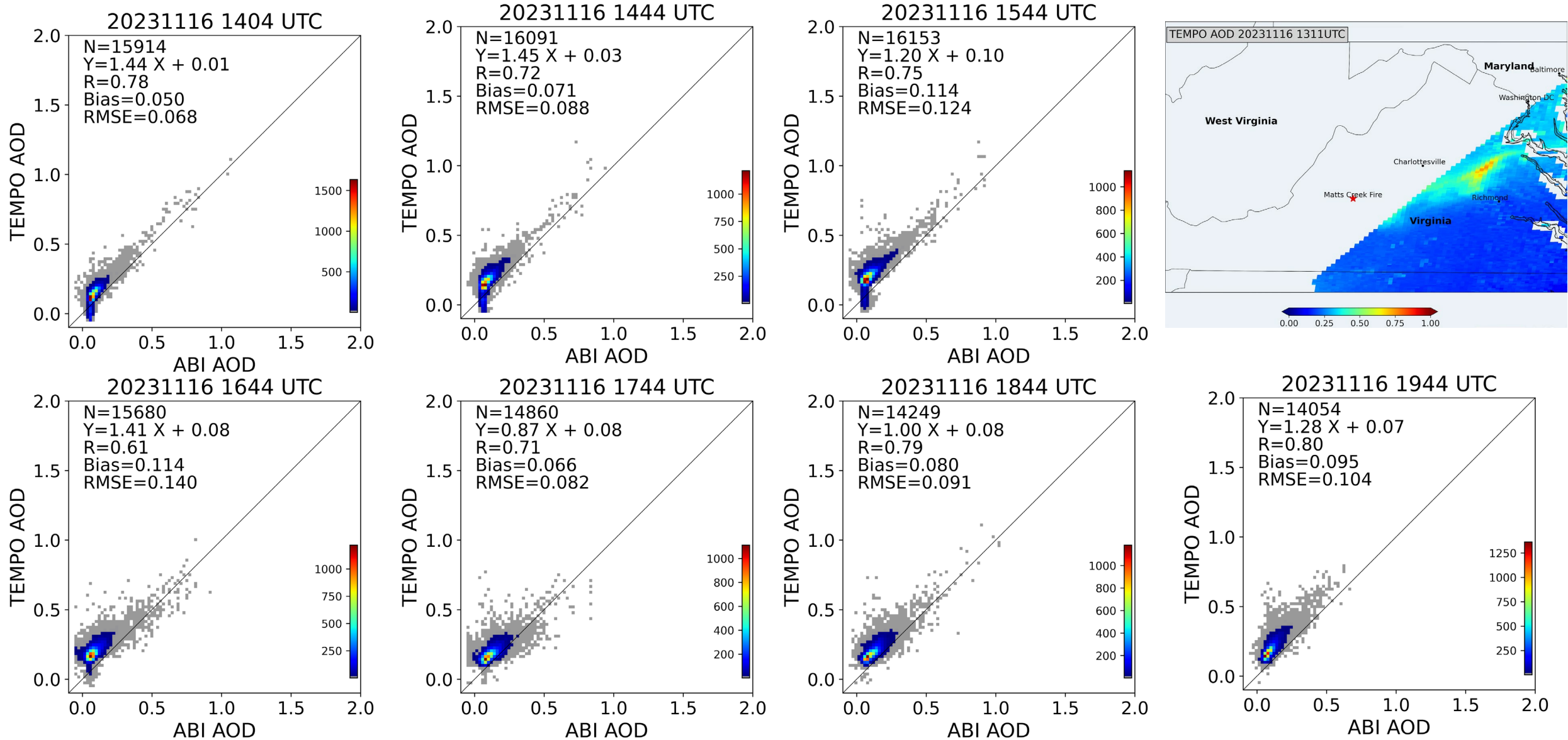
[Credit: Heesung Chong]



First Light H₂O SCD (2 August 2023)



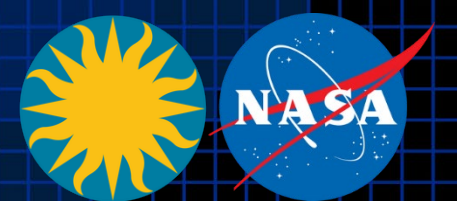
TEMPO AOD vs ABI AOD in the VA fire region



Credits: NOAA GeoXO Team, Pubu, Hai, Zigang and Shobha



Introduction to TEMPO

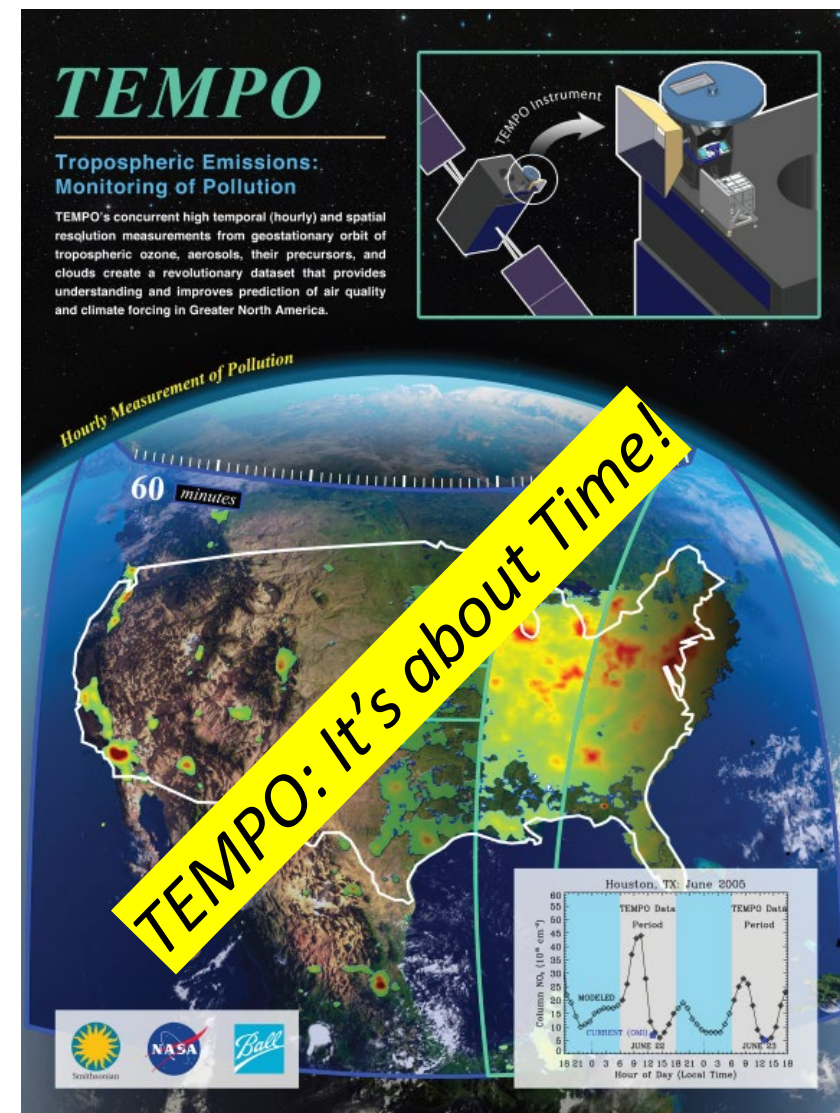


➤ NASA's first Earth Venture Instrument (EVI) selected in 2012

- ✓ **PI:** Kelly Chance, Smithsonian Astrophysical Observatory (SAO): Science team, ground systems, science data processing center
- ✓ **Instrument Project Management:** NASA LaRC → SAO (Phase E)
- ✓ **Instrument Development:** Ball Aerospace
- ✓ **Other Institutions:** NASA GSFC, NOAA, EPA, NCAR, Harvard, UC Berkeley, St. Louis U, UAH, U Iowa, Sitting Bull College, RT Solutions, Carr Astronautics
- ✓ **International collaboration:** Mexico, Canada, Cuba, Korea, U.K., ESA, Spain

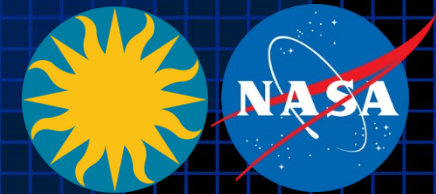
➤ NASA's first host payload

- ✓ **Mission Project Management:** NASA LaRC
- ✓ **Host Satellite Provider:** Maxar Technologies
- ✓ **Satellite Host:** Intelsat (IS-40e)
- ✓ **Launch:** SpaceX



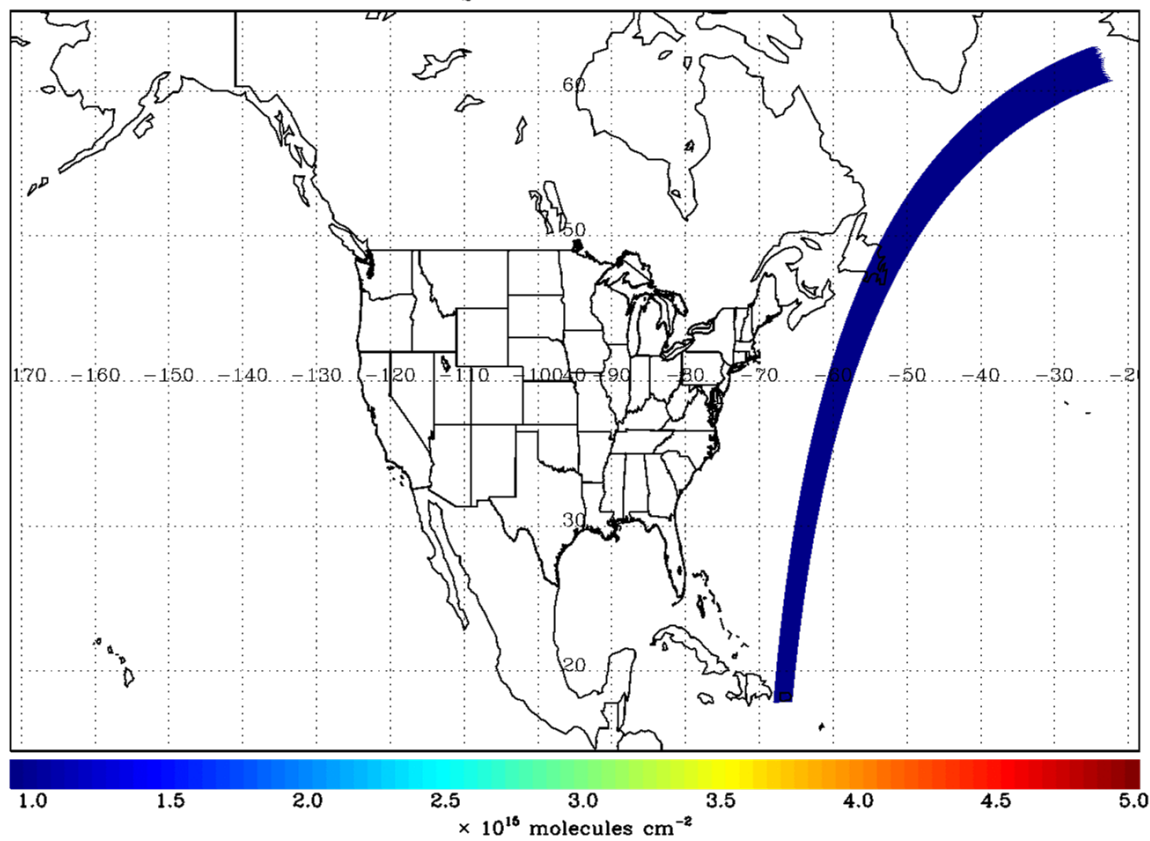


TEMPO Operation



➤ Operate on geostationary communications satellite Intelsat 40e (IS-40e) at 91° W

TROPOMI NO₂ in 2018 over TEMPO FOR



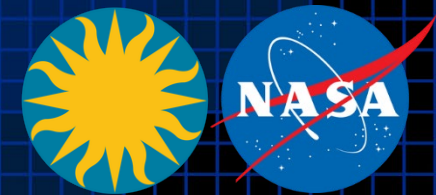
- Field of regard is optimized to cover both Puerto Rico and Canadian tar sands.
- S5p-TROPOMI NO₂ product oversampled by Kang Sun.

- **Nominal:** Scan Field of Regard (FOR) in 1 hour
 - ~ 2K N/S pixels × ~1200 steps/hr
 - 2 × 4.75 km² @center of FOR
- **Optimized scan:** in the early morning and late afternoon, daylight portion, higher temporal resolution (~40 mins)
- **Special Observations (up to 25%):**
 - ✓ **High-time scan:** selected portion at higher temporal res. (e.g., ≤ 10 mins)
 - ✓ Oversample to effectively increase spatial resolution
 - ✓ Change FOR
 - ✓ No Special observations before April release

Request special observation → https://weather.ndc.nasa.gov/tempo/green_paper.html



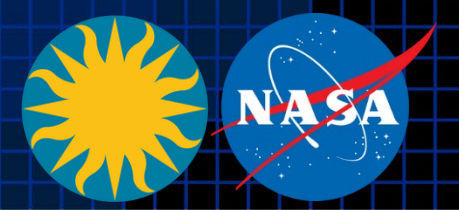
TEMPO Software/Algorithm Teams



Operational Algorithm	Personnel
Instrument Operation Center (IOC) including Raw-L0	John Davis
L0-1b	Heesung Chong, John Houck, Weizhen Hou, Xiong Liu, Dave Flittner, Jim Carr
Ozone profile	Junsung Park, Xiong Liu
Total ozone	GSFC / Junsung Park + Xiong Liu
Nitrogen dioxide	Caroline Nowlan, Gonzalo González Abad
Formaldehyde	Gonzalo González Abad, Caroline Nowlan
Clouds	Huiqun (Helen) Wang, Eun-Su Yang, Alexander Vasilkov, Joanna Joiner
Science Data Processing Center Operational Implementation & Processing Pipeline	John Houck



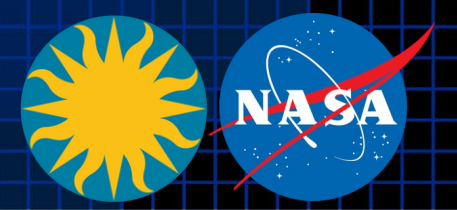
Science Algorithms



- **Launch-ready Science Data Processing Center (SDPC) V4 software completed in Mar 2023**
- **Algorithm mostly based on OMI heritage algorithms except for new L0-1b processor including Imaging Navigation and Registration (INR) using GOES-R by Carr Astronautics**
- **SAO trace gas algorithm (HCHO, NO₂): spectral fitting to derive Slant Column Densities (SCDs), calculate air mass factor (AMFs) and derive Vertical Column Densities (VCDs)**
 - ✓ NO₂ requires stratospheric/tropospheric separation based on spatial filtering method (Geddes et al., 2018)
- **Cloud algorithm: SAO O₂-O₂ fitting + NASA GSFC's O₂-O₂ cloud at ~477/466 nm**
- **Total ozone algorithm: heritage TOMS V8.5, using ozone absorbing and non ozone absorbing pairs to derive total ozone column**
- **Ozone profile algorithm: heritage SAO OMI O₃ profile, using 290-340, 540-650 nm, retrieve O₃ profile at 24 layers, including total, stratospheric, tropospheric, and 0-2 km O₃**
- **Main L1-2 algorithms updates include:**
 - ✓ NASA GMAO's GEOS-CF trace gas profiles and meteorology
 - ✓ Hourly resolved monthly mean Geometry-dependent Lambertian Equivalent Reflectivity (GLER) climatology

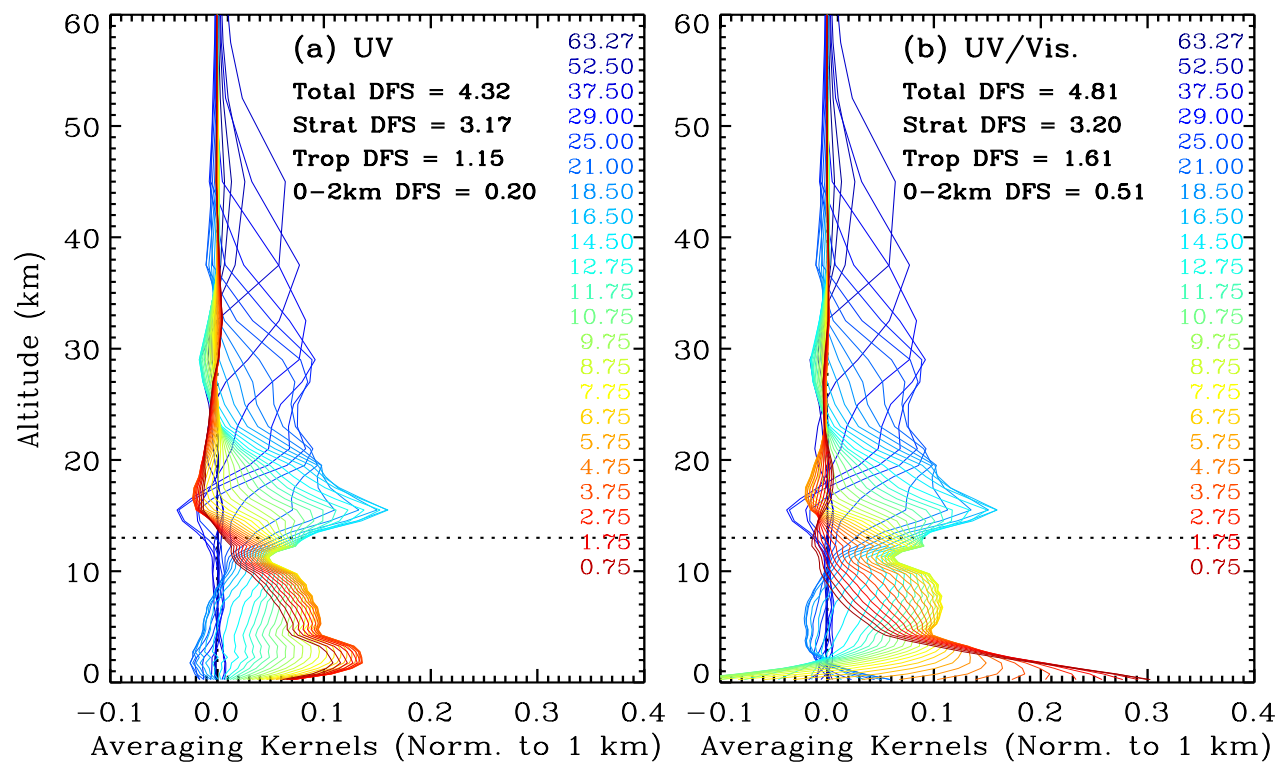
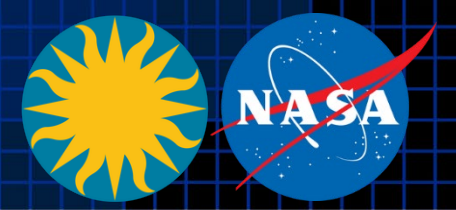


First Light NO_2 (2 August 2023)





Including Visible to Improve Tropospheric Ozone Retrieval Sensitivity

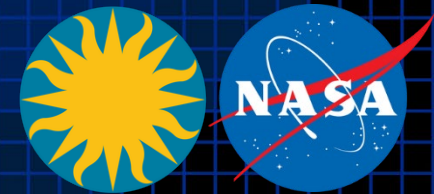


- This example is for solar zenith angle =25, viewing zenith angle 45, relative azimuthal angle 86, Signal to noise Ratio (SNR) with 4 pixels coadded
- Add visible to improve retrieval sensitivity in the lower troposphere and help separate free tropospheric O_3 from boundary layer O_3
- Under ideal conditions: 3-5 total Degree of Freedom for Signal (DFS) with up to ~1.5 in the troposphere, and up to ~0.5 DFS in 0-2 km

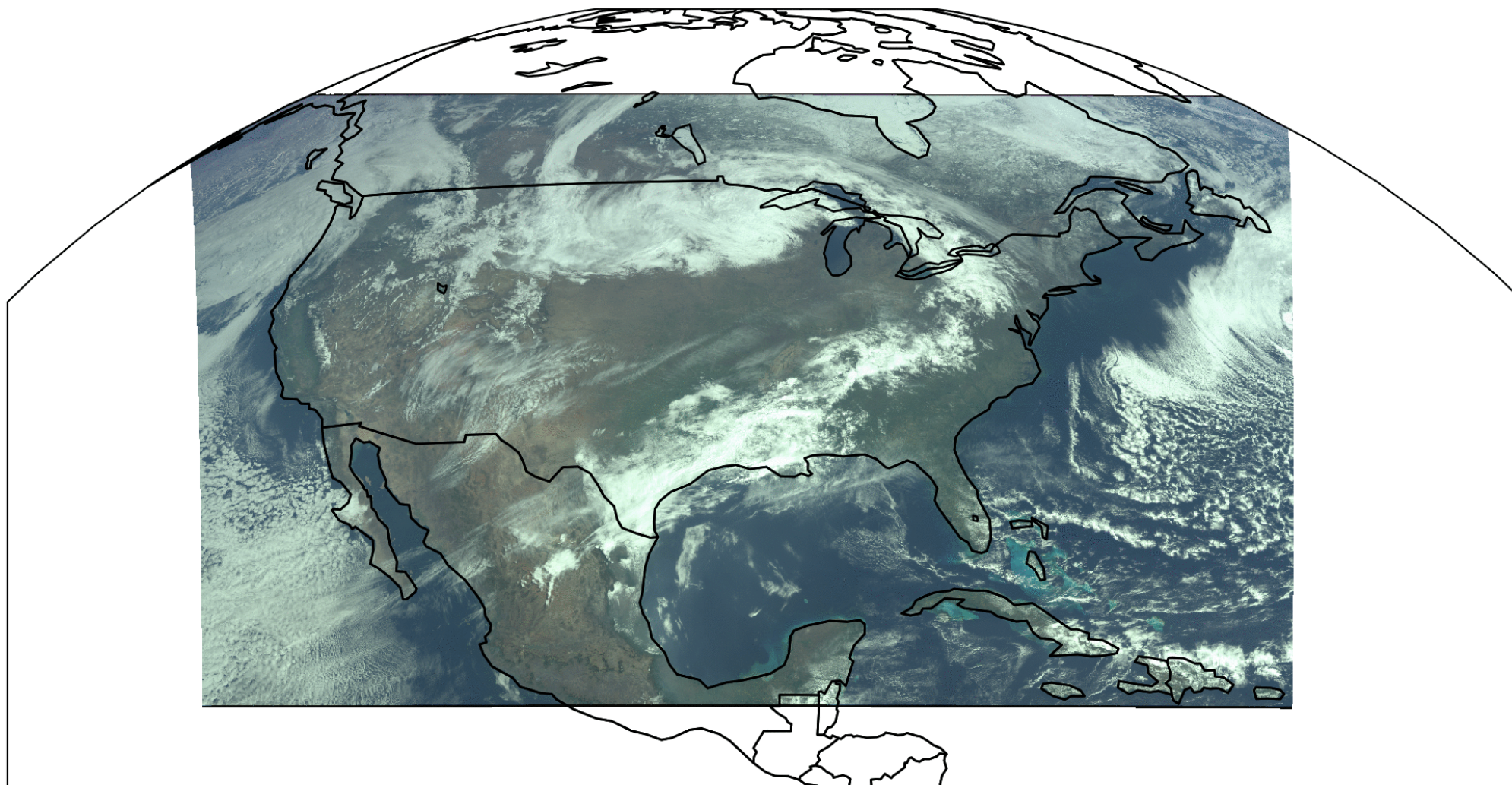
- Adapted from OMI (Liu et al., 2010): Spectral fitting + VLIDORT + Optimal Estimation (OE) from Fitting windows: 293-345 nm, 540-650 nm
- Retrieve partial O_3 columns at ~24 layers (bottom layer is 0-2 km above the surface) as well as total, stratospheric, and tropospheric O_3 columns, other trace gases, and auxiliary parameters.
- A priori: a combination of tropopause-based climatology (Bak et al., 2013) with diurnally-resolved GEOS-CF data



TEMPO Observation of Solar Eclipse



April 08, 2024
16:03:44 UTC (Scan 007)



[Credit: Heesung Chong]