Tropospheric Emissions:
Monitoring of Pollution

TEMPO

TEMPO Level 2

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…

Smithsonian Astrophysical Observatory

Joint Geostationary Science Team Meeting
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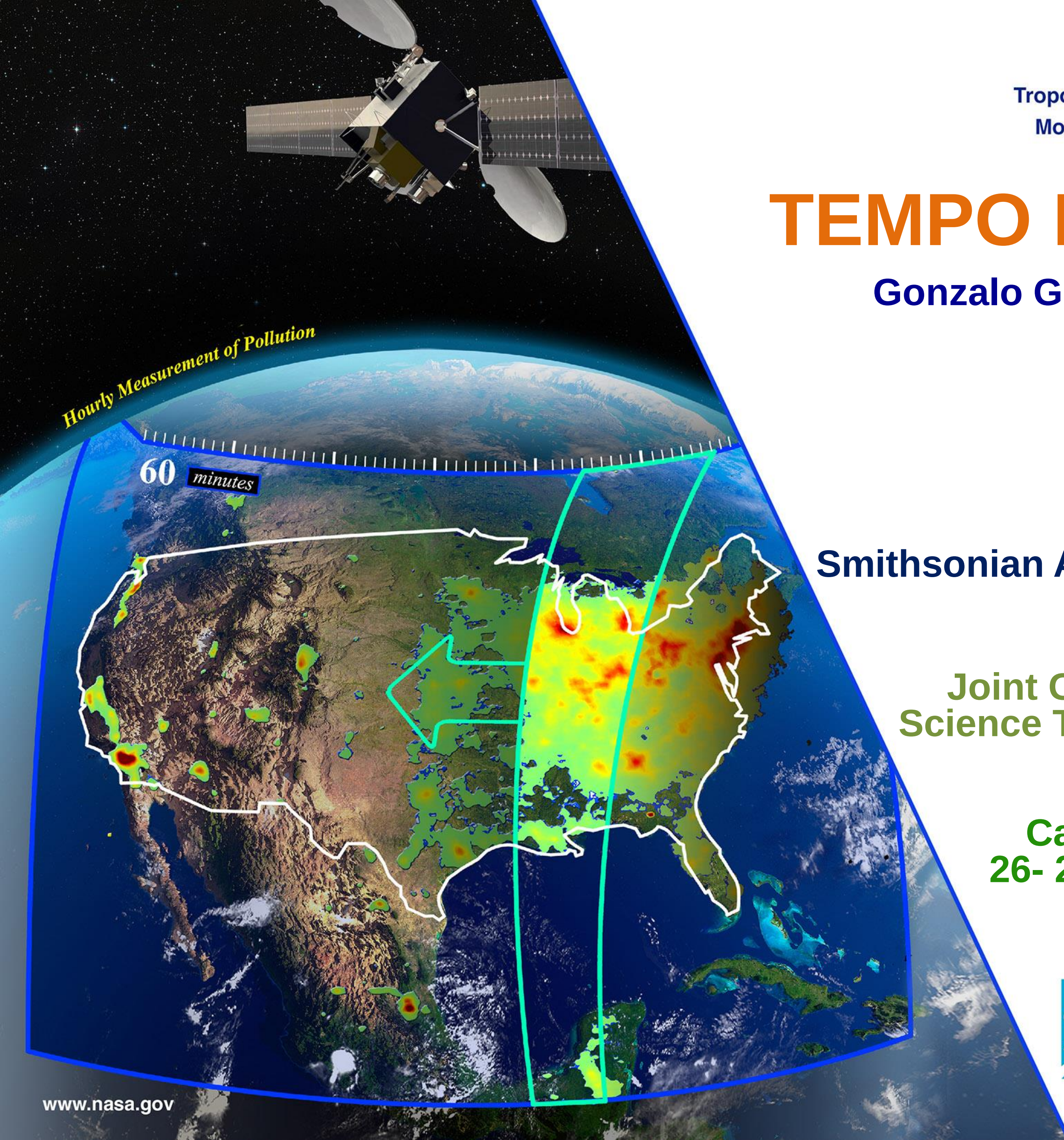

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Talk outline

- Level 2 teams
- Baseline and threshold data products
- Retrieval methods:
  - Ozone profile
  - Trace gas (nitrogen dioxide, formadelyde, ...)
  - Clouds
  - Aerosols & total ozone
- Expected performance
- Challenges
- Data product development
- Research products

L2 teams

Operational Product	Personnel
Ozone profile	Xiong Liu, Juseon Bak
Total ozone	Joanna Joiner
Nitrogen dioxide	Caroline Nowlan, Nick Krotkov, Randall Martin, Jeff Geddes, Gonzalo González Abad, Chris Chan Miller
Formaldehyde	Gonzalo González Abad, Caroline Nowlan, Chris Chan Miller
Cloud properties	Joanna Joiner
Aerosols	Omar Torres
Operational implementation and IT support @ Smithsonian Astrophysical Observatory Science Data Processing Center (SDPC) by John Houck and Ewan O'Sullivan	

Baseline and threshold level 2 products

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_2CO	1.0×10^{16} molecules cm^{-2}	3 hour
Tropospheric SO_2	1.0×10^{16} molecules cm^{-2}	3 hour
Tropospheric $C_2H_2O_2$	4.0×10^{14} molecules cm^{-2}	3 hour
Aerosol Optical Depth	0.10	1 hour

- ❑ **Aerosols (AOD, SSA, AAI), SO_2, $C_2H_2O_2$ were removed from baseline products during KDPC**
  - ➢ **Use reserve to bring them back during gap period**
- ❑ **Cloud product (cloud fraction, cloud pressure): used in trace gas retrievals**

Baseline and threshold level 2 products

Level	Product	Algorithm	Major Outputs	Spa Res km^2	Freq/Size
L2	**Cloud**	OMCLDRR	Cloud fraction, cloud pressure	2.1 x 4.5	Hourly, granule
	O_3 profile	SAO O3 profile	O3 profile, total/strat/trop/0-2 km O3 column, errors, a priori, averaging kernels	8.4 x 4.5	Hourly, granule
	Total O_3	TOMS V8.5	Total O3, AI, cloud frac	2.1 x 4.5	Hourly, granule
	NO_2	SAO trace gas Washington/BU strat/trop sep.	SCD, strat./trop. VCD, error, shape factor, scattering weights	2.1 x 4.5	Hourly, granule
	H_2CO	SAO trace gas	SCD, VCD, error, shape factor, scattering weights	2.1 x 4.5	Hourly, granule
	SO_2	SAO trace gas		2.1 x 4.5	Hourly, granule
	$C_2H_2O_2$	SAO trace gas		2.1 x 4.5	Hourly, granule
	H_2O,BrO	SAO trace gas		2.1 x 4.5	Hourly, granule
	Aerosol	OMAERUV	AAI, AOD, SSA	8.4 x 4.5	Hourly, granule
L3	**Gridded L2**	SAO L2-3	Same as L2	TBD	Daily/Monthly Hourly, scan
L4	**AQ Index**	Washington, EPA	Air quality index	TBD	Hourly, scan
	UVB	OM UVB	UV irradiance, erythemal irradiance, UV index	TBD	Hourly, scan

Baseline/launch retrieval methods

NO_2, H_2CO, SO_2, $C_2H_2O_2$ vertical columns

- Direct fitting to TEMPO radiances (e.g., heritage from OMI OMHCHO)
- AMF-corrected reference spectra, Ring effect, etc.
- NO_2 strat./trop. separation (STS) adapted from OMI

O_3 profiles and tropospheric O_3

- SAO OE-based ozone profile method developed for GOME and OMI
- Add visible to improve retrieval sensitivity in the lower troposphere
- May be extended to SO_2, especially volcanic SO_2

TOMS-type total ozone retrieval (OMTO3) included for heritage

Aerosol products based on OMAERUV: AOD, AAOD, Aerosol Index

- Advanced/improved products likely developed @ GSFC, U. Iowa, NOAA

Cloud Products from OMCLDRR: CF, CTP

- Advanced/improved products likely developed @ GSFC

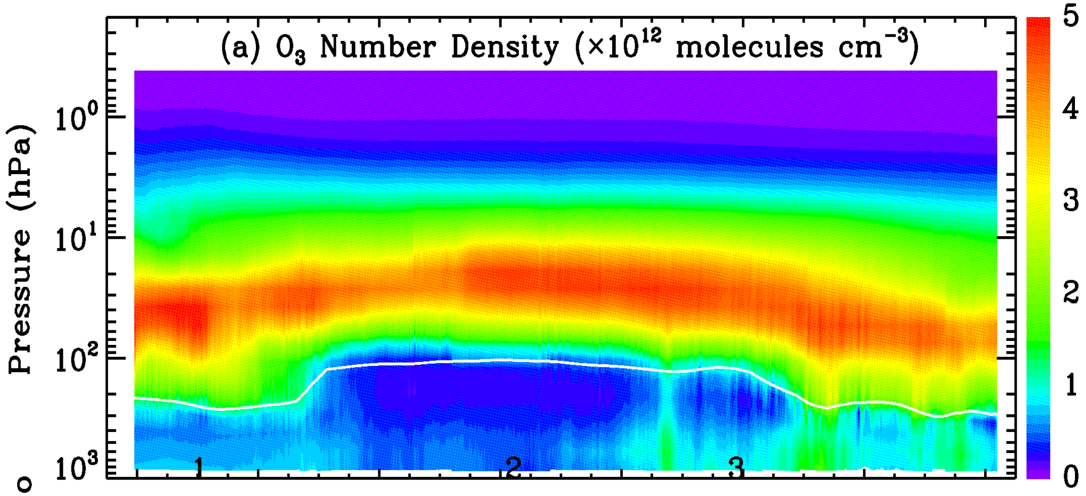
UVB research product based on TOMS/OMI heritage (FMI, GSFC)

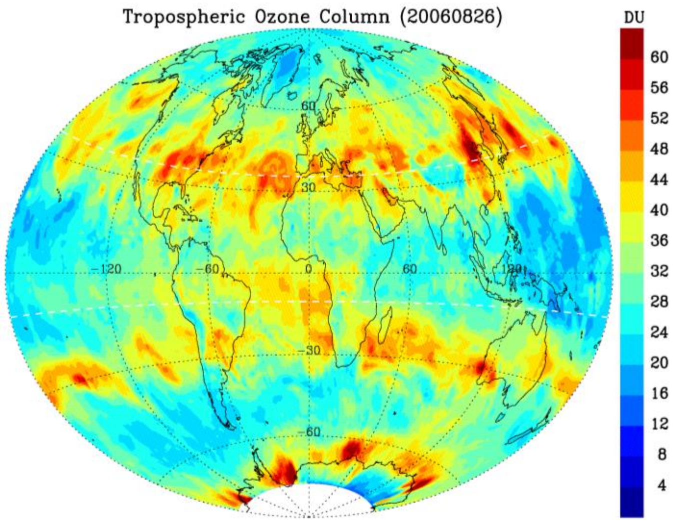
TEMPO Retrieval Sensitivity Studies

- **Performed RTM simulations of TEMPO radiance spectra and optimal estimation based retrieval sensitivity studies for determining instrument requirements & verifying instrument performance.**
  - **VLIDORT: adapted from previous GEO-CAPE tools, with interfaces for viewing geometry, built-in cross sections, pre- and after- convolution, HITRAN line by line calculations, aerosol profiles and plumes, scattering clouds, IPA, Koelemeijer GOME surface albedo database or input surface reflectance spectra**
  - **Hourly fields of GEOS-Chem model fields over TEMPO field of regard for 12 days (1 day/month) up to SZA 80° → ~90,000 simulations with 10 gases (O_3, NO_2, H_2CO, SO_2, $C_2H_2O_2$, H_2O), BrO, OClO, O_2, O_4, 6 types of aerosols, water/ice clouds**
  - **TEMPO SNR model: account for optical transmission and grating efficiency, including shot, dark current, RTN, readout, quantization, smear, CTE noise terms**
  - **Climatological a priori: climatological for O_3, unconstrained for other trace gas VCDs, consistent with current algorithms**
  - **Optimal estimation to perform retrieval sensitivity and error analysis**

Retrieval methods: Ozone profile

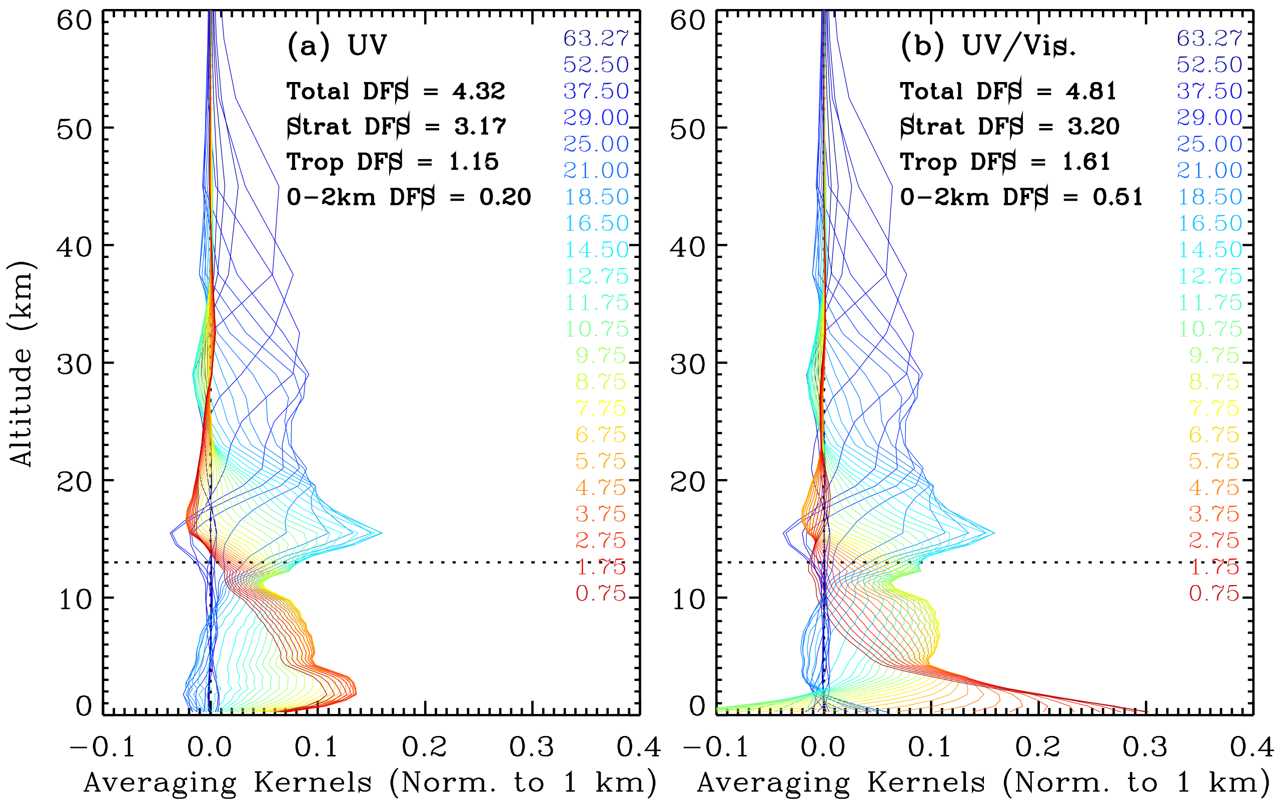
- **Adapted SAO OE-based algorithm developed for GOME and OMI (Liu et al., 2005, 2010) to retrieve <u>partial ozone columns at ~24 layers as well as total, stratospheric, tropospheric, and 0-2 km ozone columns</u> from normalized radiance in the UV (290-345 nm) and visible (540-650 nm)**
  - Climatological a priori: tropopause-based O_3 profile climatology (Bak et al., 2013) or diurnally resolved O_3 climatology based on the GEOS-5 nature run at 12 km x 12 km
  - Include retrieval a priori, retrieval error, retrieval error covariance matrix, retrieval averaging kernels





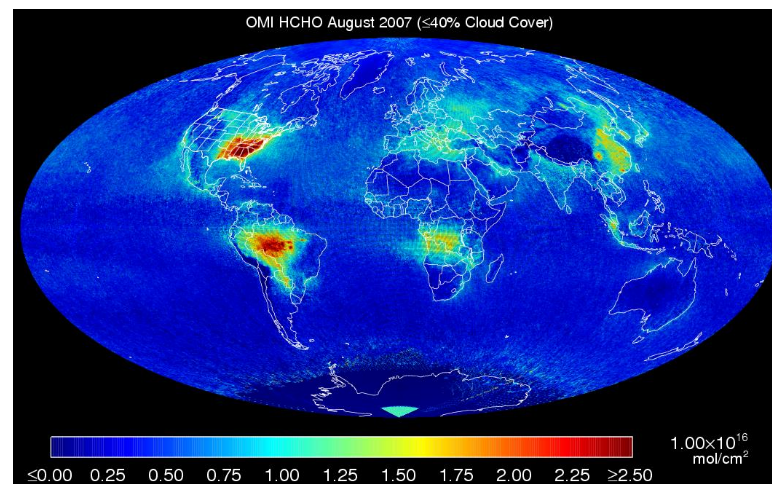
Retrieval methods: Ozone profile

- Add visible to improve retrieval sensitivity in the lower troposphere
- Combine MODIS albedo/BRDF database at high spatial resolution with existing spectral albedo libraries to improve the characterization of surface albedo spectra
- Time consuming due to on-line radiative transfer calculations: perform retrievals at 8.4 x 4.5 km^2, data latency within 24 hours

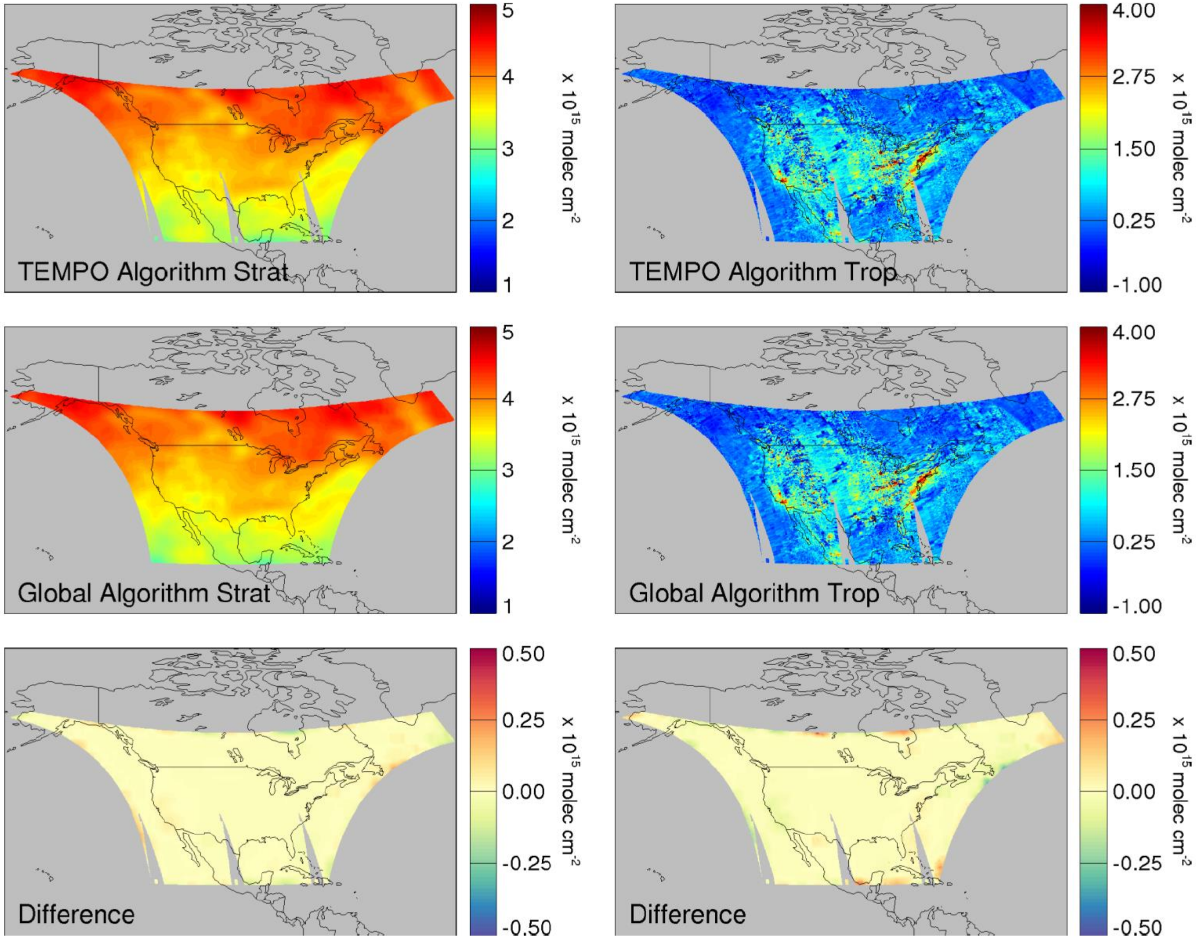


Retrieval methods: trace gas

- **Adapted from SAO two-step OMI trace gas algorithm and NASA NO_2 stratospheric/tropospheric separation (STS) algorithm to retrieve VCDs of trace gases (e.g., NO_2, H_2CO, H_2O, SO_2, $C_2H_2O_2$) from normalized radiance in selected spectral windows**
  - Direct fitting to TEMPO radiances (e.g., OMHCHO) to derive SCD
  - Air Mass Factor (AMF) from diurnally resolved trace gas climatology based on the GEOS-5 nature run at 12 km x 12 km, surface albedo climatology, TEMPO cloud products, look-up table of scattering weights
  - Product includes SCD, VCD, retrieval errors, profile shape, scattering weights, AMFs. NO2 product includes separate strat./trop. SCDs/VCDs



Retrieval methods: NO_2 Strat./Trop. Separation (STS)



J. Geddes (BU) and R. Martin (Washington Univ.) adapted NASA OMI NO_2 STS algorithm to TEMPO (limited domain) finding overall good performance and small errors of ~2.0E14 molecules at the edge minimized with LEO support

Retrieval methods: Clouds

- **Adapted from OMCLDRR to retrieve effective cloud fraction and optical centroid pressure (OCP) from TEMPO normalized radiances in ~346-354 nm**
  - Rotational Raman Scattering (RRS) cloud algorithm developed for OMI (OMCLDRR) by **Joiner et al. at GSFC**
  - RRS by air molecules produces filling and depletion effects in radiance spectrum called the Ring effect, cloud/aerosol reduces RRS
  - Mixed Lambertian Equivalent Model (MLER): cloud/surface is assumed to be opaque Lambertian, an effective cloud fraction is used to weigh the clear and cloudy portion of a pixel
  - Effective cloud fraction is derived from a wavelength not sensitive to RRS and atmospheric RRS
  - RRS is fitted from spectral fitting, and used to derive OCP from a look-up table
- **The RRS cloud retrievals are sensitive to instrumental (e.g., stray light, dark current), geophysical effects (e.g., 3D, shadow)**
  - Backup algorithm is being developed based on absorption O_2-O_2 at 477 nm at GSFC

Retrieval methods: Aerosols and total ozone

- **Will adapt from OMI's OMAERUV developed by O. Torres at GSFC to retrieve Absorbing Aerosol Index (AAI), Aerosol Optical Depth (AOD), and Single Scattering Albedo (SSA) from TEMPO normalized radiances at ~354 and 388 nm.**
  - Uses the sensitivity of near-UV observations to particle absorption to retrieve aerosol absorption properties in conjunction with the aerosol extinction optical depth
  - Assume three aerosol types (refractive index & size distribution): carbonaceous, desert dust, and urban/industrial particulate
  - Aerosol height climatology from CALIPSO (Cloud-Aerosol Lidar with Orthogonal Polarization) measurements
  - Surface albedo climatology
  - Four pixels might be used for cloud clearing, so the product resolution is at 8.4 x 4.5 km^2.
- **Adapted from OMI TOMS-type V8.5 (OMTO3) to retrieve total ozone, surface reflectivity, AAI, from TEMPO normalized radiances at a few wavelengths (e.g., 317/331 nm, 331/360 nm)**

Expected performance

Table 1.
Key TEMPO instrument parameters based on the latest design as of February 2016 for a geostationary satellite at 100°W. The signal to noise ratio is the average value over the specific retrieval windows for the nominal radiance spectrum. IFOV is Instantaneous Field of View at 36.5°N, 100°W. MTF is Modulation Transfer Function at Nyquist.

Parameter		Value	Parameter	Value
Mass		148 kg	Spectral range	290–490 nm, 540–740 nm
Volume		1.4 × 1.1 × 1.2 m	Spectral resolution & sampling	0.57 nm, 0.2 nm
Avg. operational power		163 W	Albedo calibration uncertainty	2.0% λ-independent, 0.8% λ-dependent
Average Signal to Noise [hourly @ 8.4 km x 4.4 km]	O_3:Vis (540–650 nm)	1436	Spectral uncertainty	$<$ 0.1 nm
	O_3: UV (300–345 nm)	1610	Polarization factor	$\leq$2% UV, $<$10% Vis
	NO_2: 423–451 nm	1771	Revisit time	1 h
	H_2CO: 327–356 nm	2503	Field of regard: N/ S × E/W	4.82° × 8.38° (greater North America)
	SO_2: 305–345 nm	1797	Geo-location Uncertainty	2.8 km
	$C_2H_2O_2$: 420–480 nm	1679	IFOV: N/S × E/W	2.1 km × 4.4 km
	Aerosol: 354, 388 nm	2313	E/W oversampling	5%
	Clouds: 346–354 nm	2492	MTF of IFOV: N/S × E/W	0.19 × 0.36

Zoogman et al., 2017, JQSRT, TEMPO Overview

*** SNR are for 4 pixels coadded as requirements are derived from coadding 4 pixels at 8.4 x 4.5 km^2!**

Expected performance

Table 3.
Statistics (mean and 1σ) of retrieval precisions and errors for various products, and the percentage of scenarios meeting the requirements (MR).

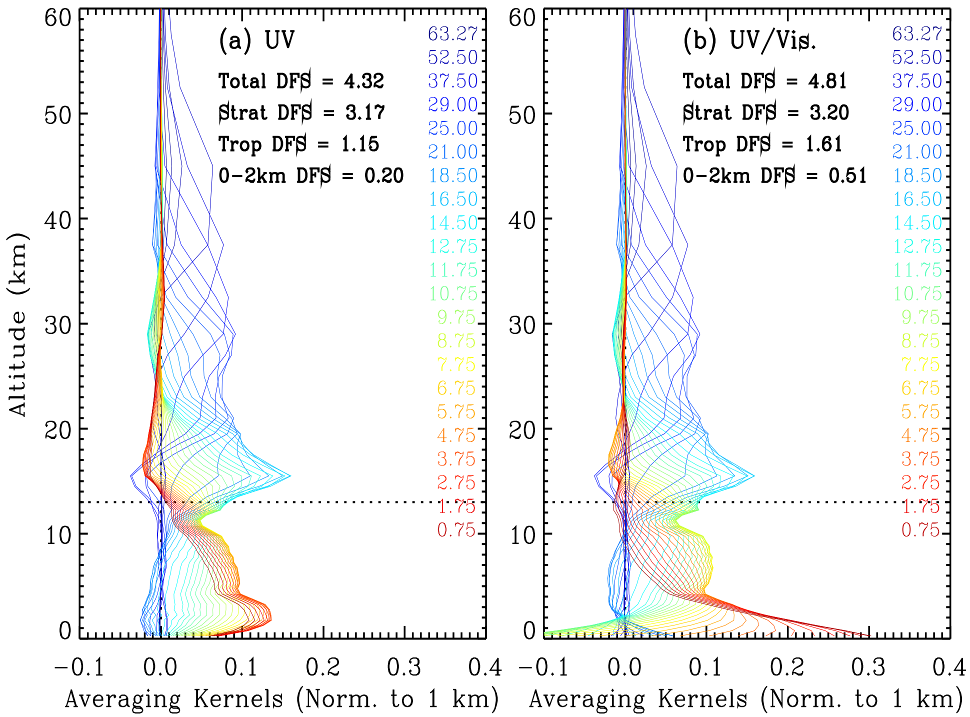
Product[a]	Precision	Total errors	Meets reqs. (%)
UV total O_3	0.32 ± 0.08	0.72 ± 0.08	100
UV trop. O_3	3.05 ± 0.71	6.38 ± 1.98	98.3
UV 0-2 km O_3	2.59 ± 0.70	8.86 ± 1.53	78.2
UV/Vis total O_3	0.30 ± 0.07	0.54 ± 0.13	99.4
UV/Vis trop. O_3	3.04 ± 0.90	5.21 ± 1.72	98.9
UV/Vis 0–2 km O_3	3.29 ± 0.71	7.93 ± 1.41	92.8
NO_2 ($\times 10^{15}$)	0.30 ± 0.08	0.36 ± 0.20	98.4
H_2CO ($\times 10^{16}$)	0.38 ± 0.10	0.42 ± 0.13	100
$C_2H_2O_2$ ($\times 10^{14}$)	4.68 ± 1.56	4.75 ± 1.62	N/A
SO_2 ($\times 10^{16}$)	1.09 ± 0.49	1.86 ± 1.04	N/A

[a] The units are % for total ozone column, ppbv for tropospheric O_3 and 0–2 km O_3, and molecules cm $^{-2}$ for other trace gases.

Zoogman et al., 2017, JQSRT, TEMPO Overview

- **Clear-sky conditions**
- **O_3: fitting precision, vertical smoothing, interferences**
- **Other trace gases: fitting precision, interference. Uncertainties due to AMFs not considered.**

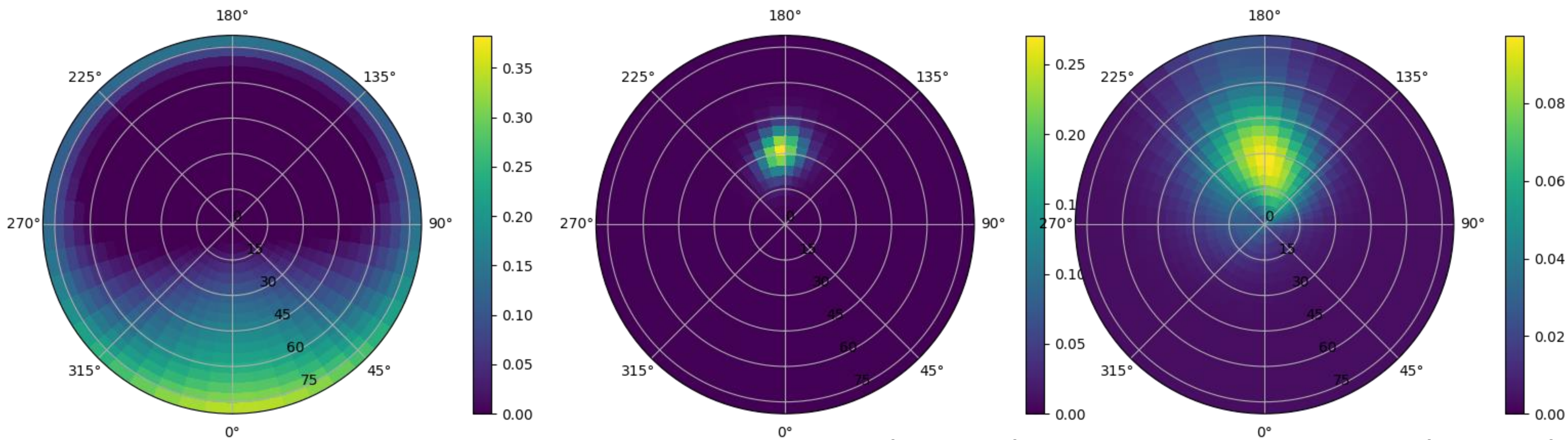
Challenges for TEMPO Ozone Profile Algorithm



- It depends on absolute radiometric calibration and consistent calibration between UV and Visible bands: requires soft calibration
- Due to the weak signal from the visible, it is critical to have good knowledge of surface albedo/BRDF spectra: MODIS albedo/BRDF+EOFS of surface albedo spectra
- For retrieval of lower tropospheric ozone, it might be important to retrieve/correct for aerosol effects (yet to be implemented).
- Retrieval is computation-demanding as it involves on-line radiative transfer calculation: we are combining PCA-RTM with look-up table correction to speed up retrievals.

Challenges: surface properties

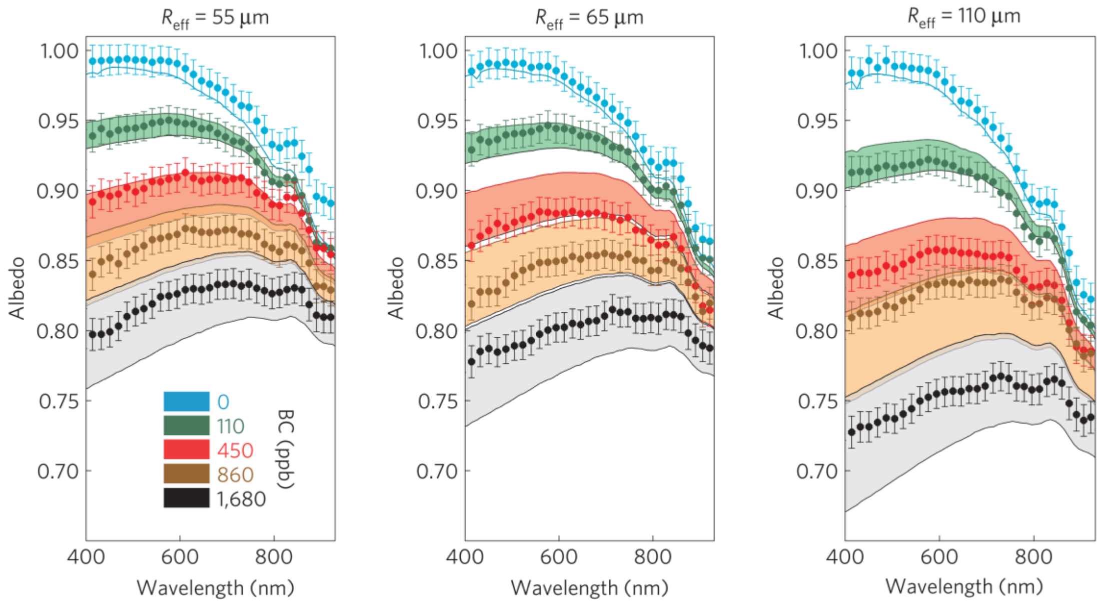
- ➢ The current baseline surface reflectance climatology is for historical reasons the OMLER dataset (Kleipool et al., 2008)
- ➢ TEMPO will ideally use surface reflectance at higher spatial resolution (OMLER is 0.5°) considering SZA dependence
- ➢ Proposed solution, derive SZA dependent Lambertian reflectance using MODIS BRDF climatology at different wavelengths



Ross thick Ocean Cox-Munk (ws=1) Ocean Cox-Munk (ws=5)

Challenges: snow/ice cover and treatment

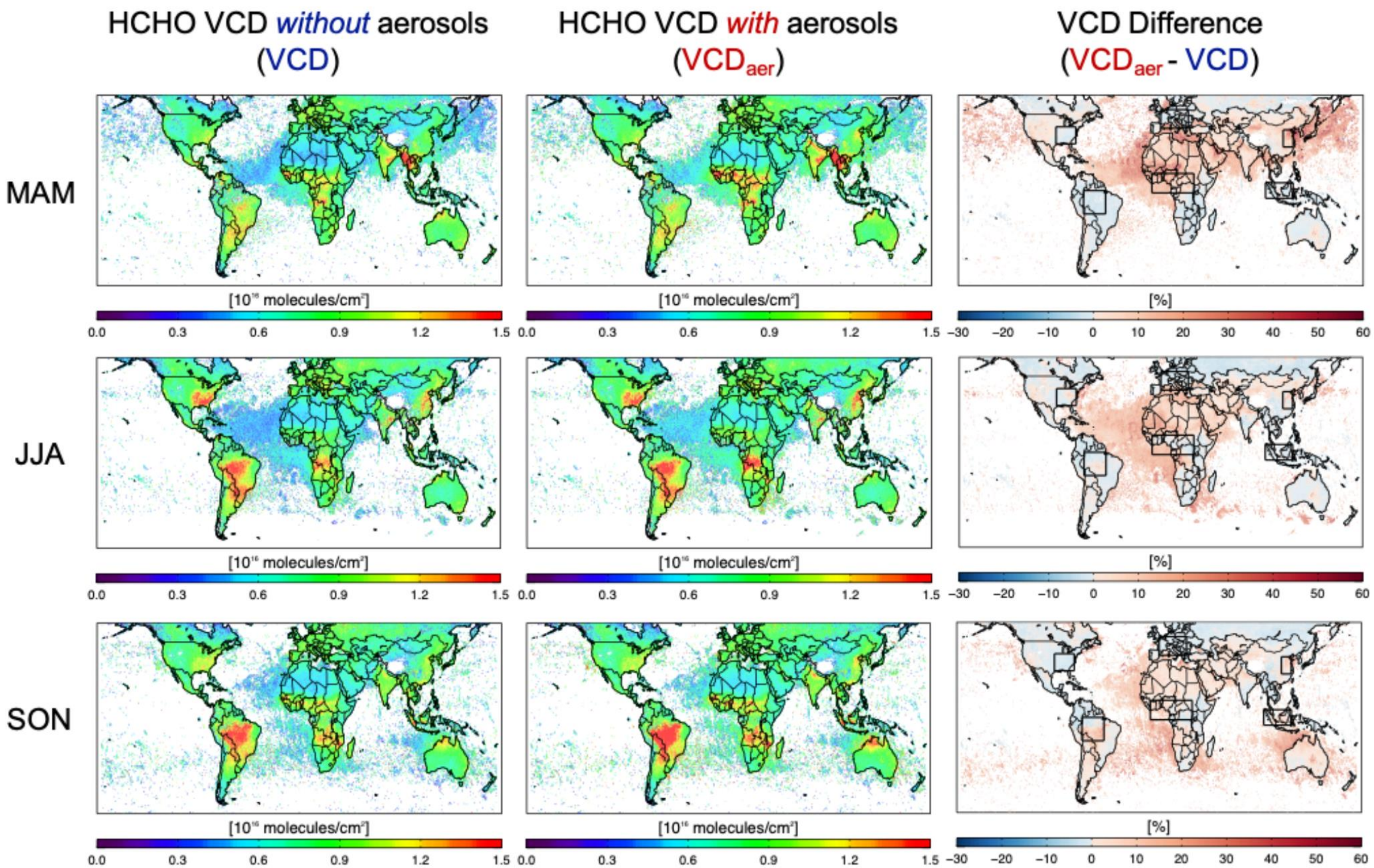
- Snow/ice information is incorporated into L1b files from the NSIDC
- Snow and ice is considered in AMF calculations assuming a constant albedo (e.g., 0.8)
- However, we know:
  - Snow and ice affect cloud retrievals
  - Snow albedos vary as function of effective radius, depth, age, contamination…
  - Snow information is not available to account for these variations



Hadley et al., 2012

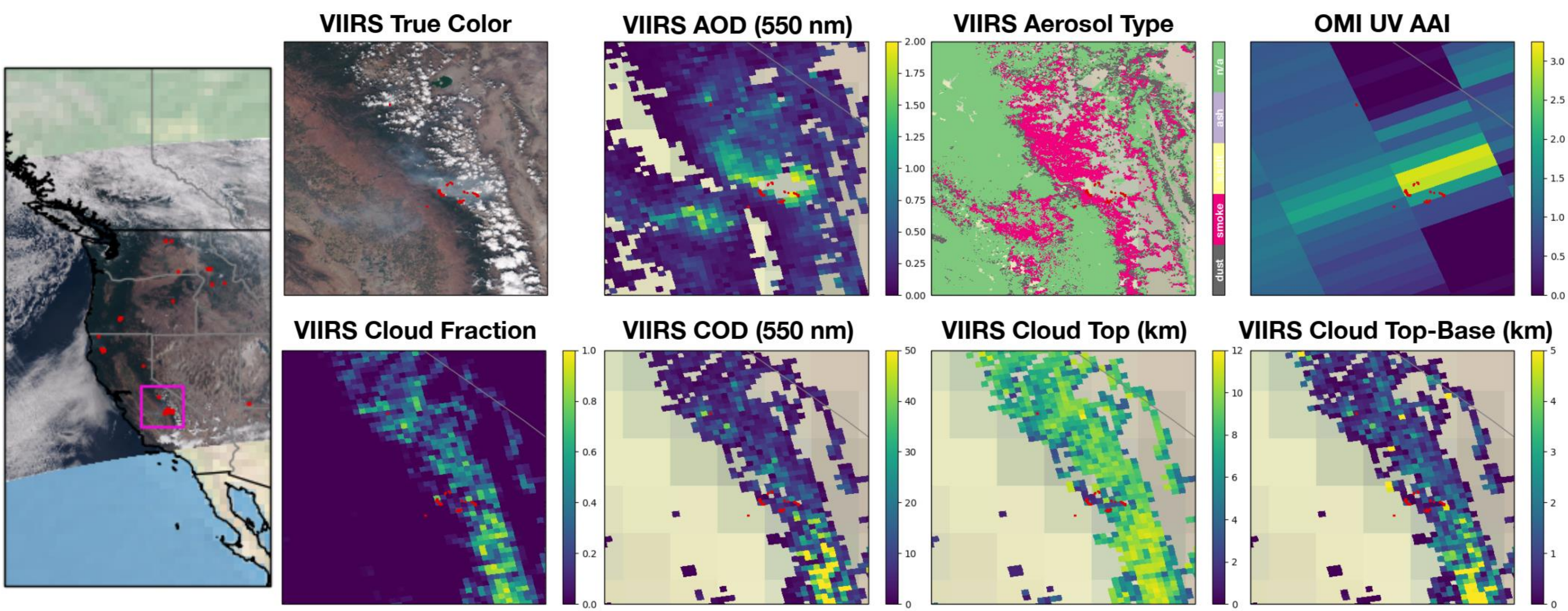
Challenges: aerosols

- TEMPO's radiative transfer (Ozone profile and trace gas AMFs doesn't consider aerosols) which significantly modify photon paths and observation vertical sensitivities



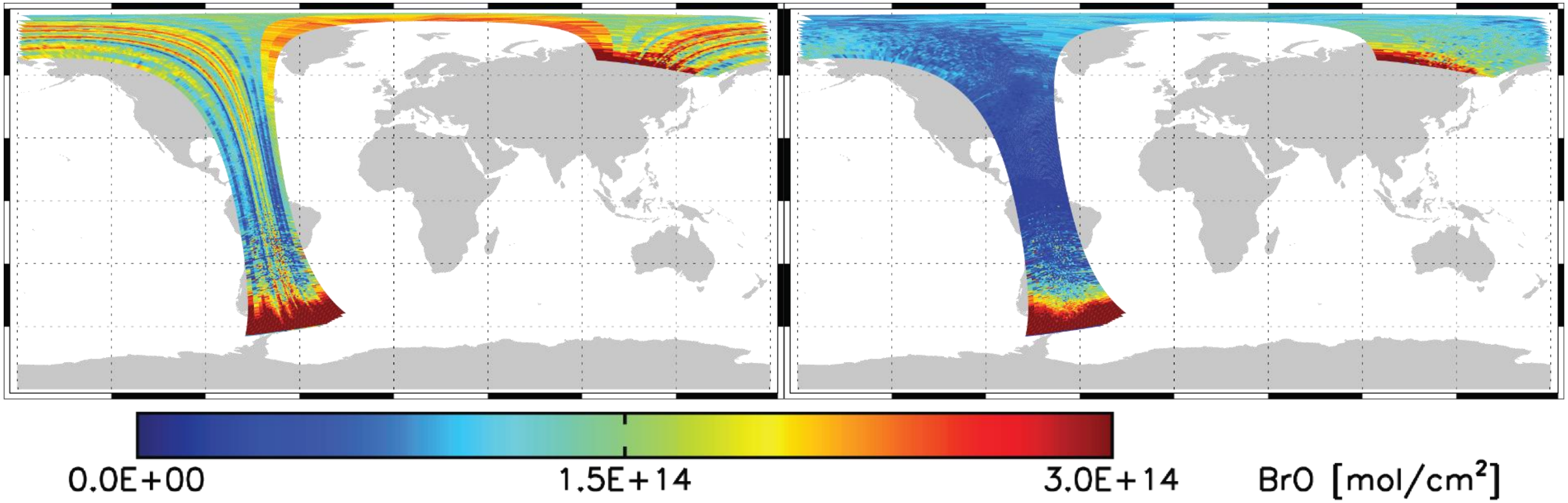
Challenges: retrieval over fires

- How to obtain consistent a-priori information about clouds, aerosols, vertical distribution, scene reflectance, ...?
- Would it be possible to exploit synergies between TEMPO, GOES-R and LEO observations?



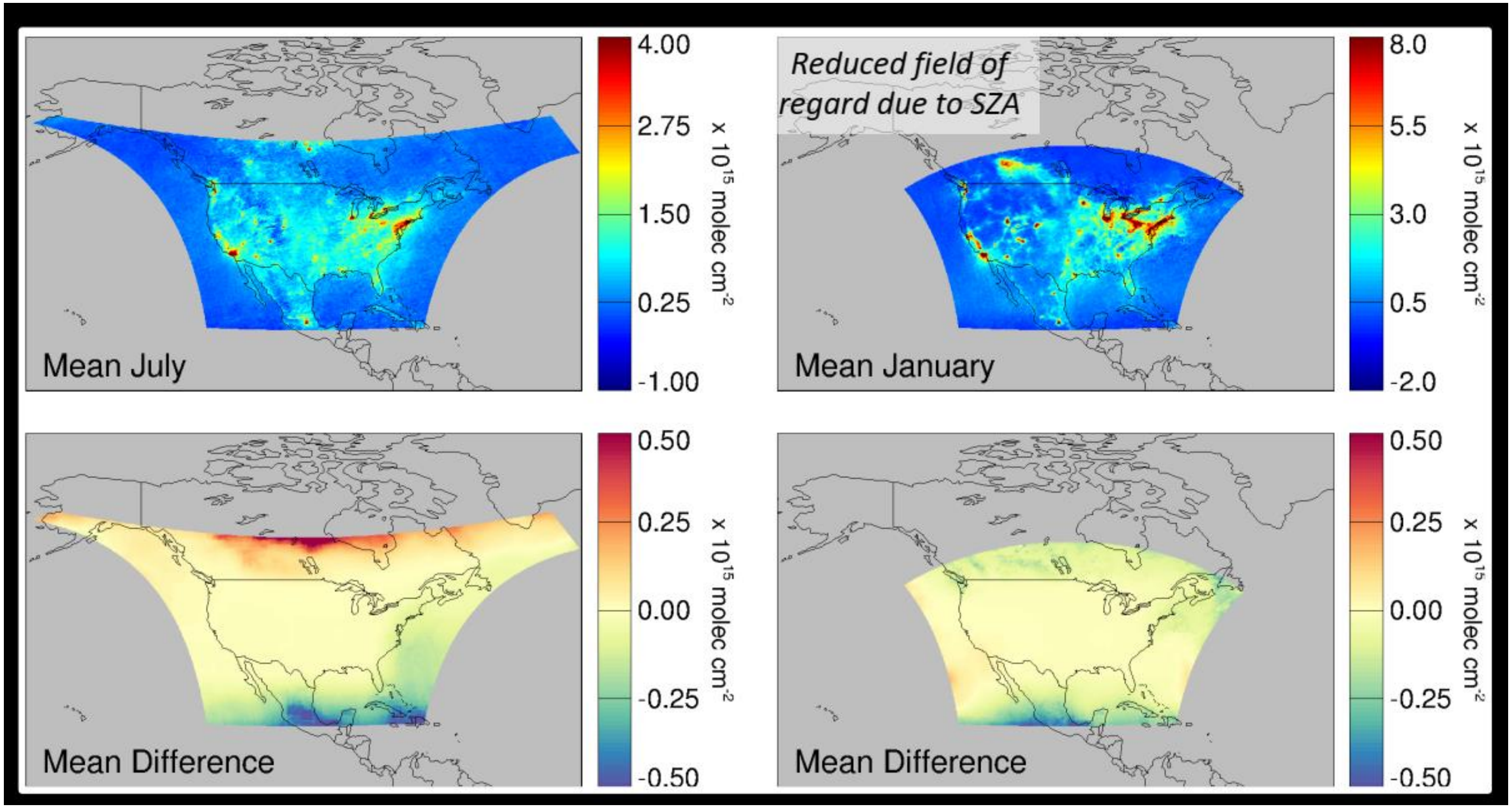
Challenges: stripes (reference sector)

- One of the strategies used to minimize the impact of stripes in retrievals of weakly absorbing species is to use a radiance reference instead of a solar irradiance in the direct fit algorithms.
- Traditionally the radiance reference has been obtained using measurements over a reference sector with small and fairly homogeneous fields of the target species.
- Will that be an option for TEMPO if needed? It is necessary to find alternative definitions of the reference sector



Challenges: strat./trop. separation

- The performance of the STS algorithm its affected near the edges of TEMPO's field of regard. To avoid this issue context information from LEO observations is provided. NRT NO_2 product will use a monthly climatology instead of LEO observations.

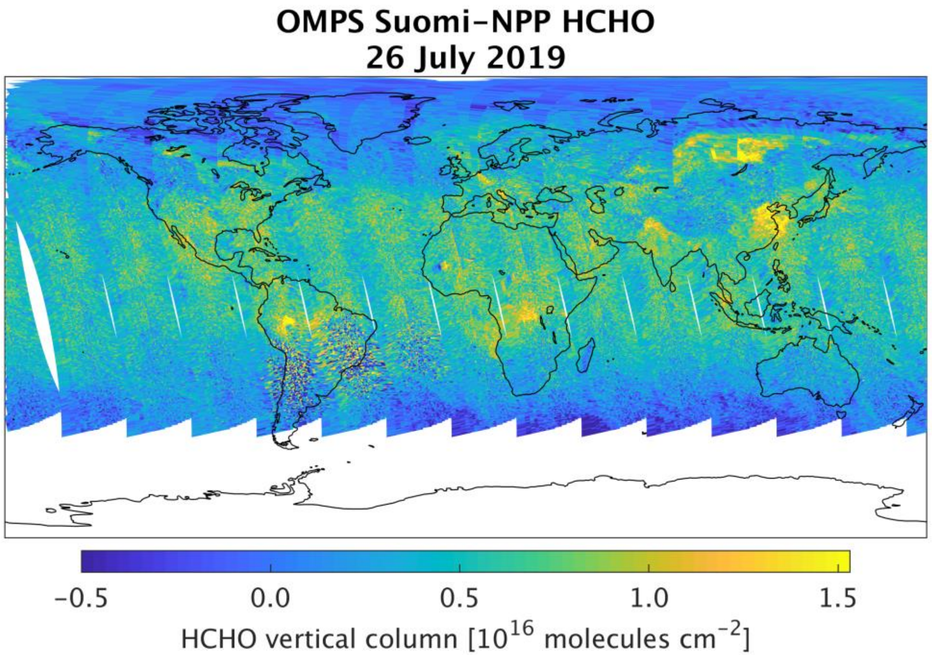


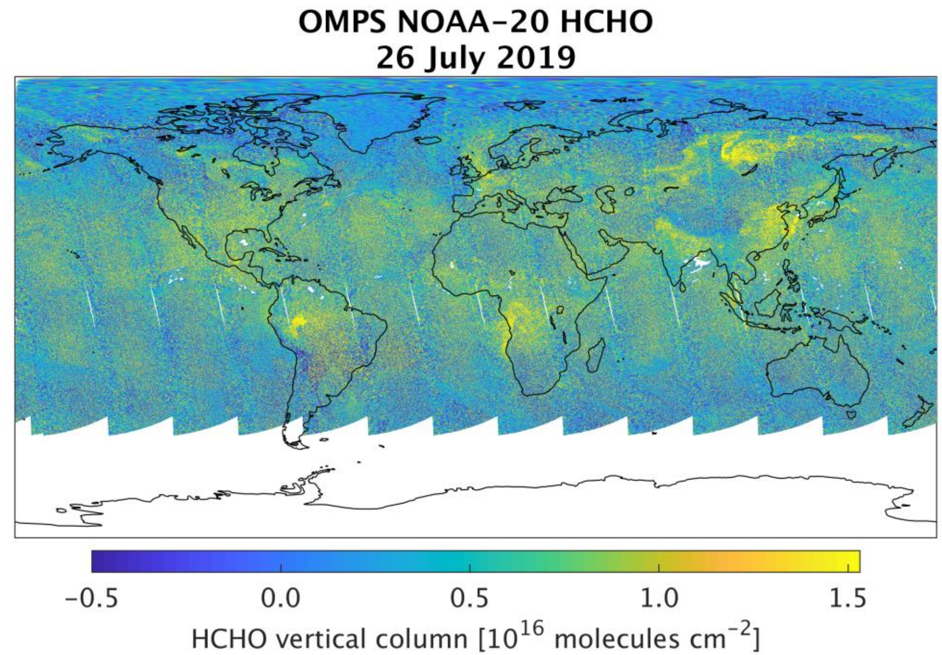
Data product development

- Version 1 ready (mostly OMI algorithms adapted for TEMPO) has been implemented and being tested using synthetic data.
- Version 2 to be delivered by April 2020 with updates in ancillary (trace gas and surface albedo climatologies, LUT) data and algorithm physics.
- Science team members develops/updates and test algorithm features that are later on integrated in the operation pipeline by the SDPC team (John and Ewan).

Data product development

- Spectral fitting trace gas algorithm is being thoroughly tested after been adapted to process OMI, OMPS, and TROPOMI observations (SAO MEaSUREs HCHO, H_2O and CHOCHO project)





Research products

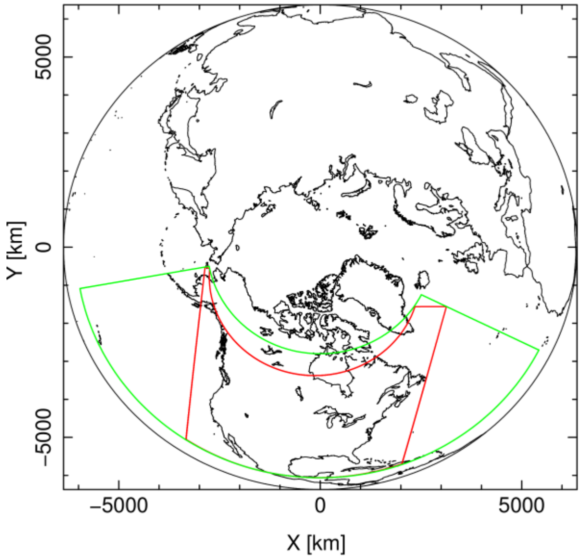
- **TEMPO research products will greatly extend science and applications**
  - H_2O, BrO, OClO, IO, and volcanic (SO_2 plume height and VCD)
  - Additional/improved cloud with O_2-O_2 bands or O_2-B bands
  - Additional aerosol products from hyperspectral spectra, O_2-B and O_2-O_2 bands, and TEMPO + GOES-R synergy at @U Iowa, GSFC, NOAA
  - Vegetation products: solar Induced fluorescence (SIF)
  - Diurnal out-going shortwave radiation and cloud forcing
  - City lights
  - Higher-level products: Near-real-time pollution/AQ indices, UVB/UV index
  - Data fusion possibilities between TEMPO, GeoCarb, GLIMR, and GOES-R sensors (carbon cycle, ocean, cloud, aerosols, ice/snow, land cover, lightning…)

Extra/back up slides

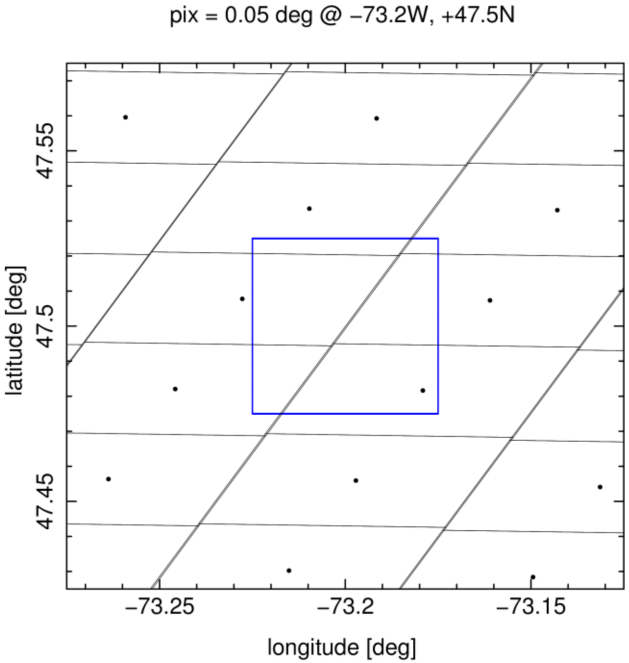
Retrieval methods: re-gridding algorithm

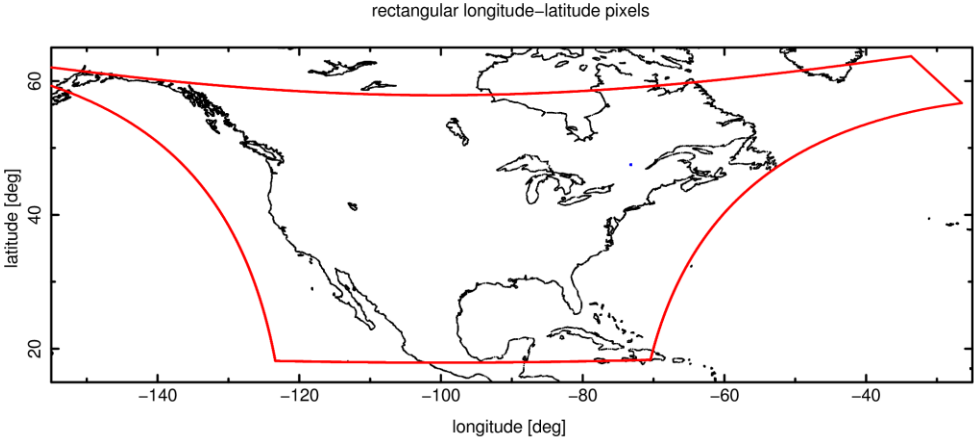
- L3 product involves re-gridding selected L2 product variables onto a longitude-latitude grid with square pixels.
  - Each L3 pixel value is an area-weighted (and also uncertainty-weighted) mean of overlapping L2 pixel values, filtered to exclude bad data.
  - Each L3 product covers a single full east-west scan.
- Relatively inexpensive calculation – geometry & averaging.
  - Geometric projections available from OTS libraries.

Retrieval methods: re-gridding algorithm



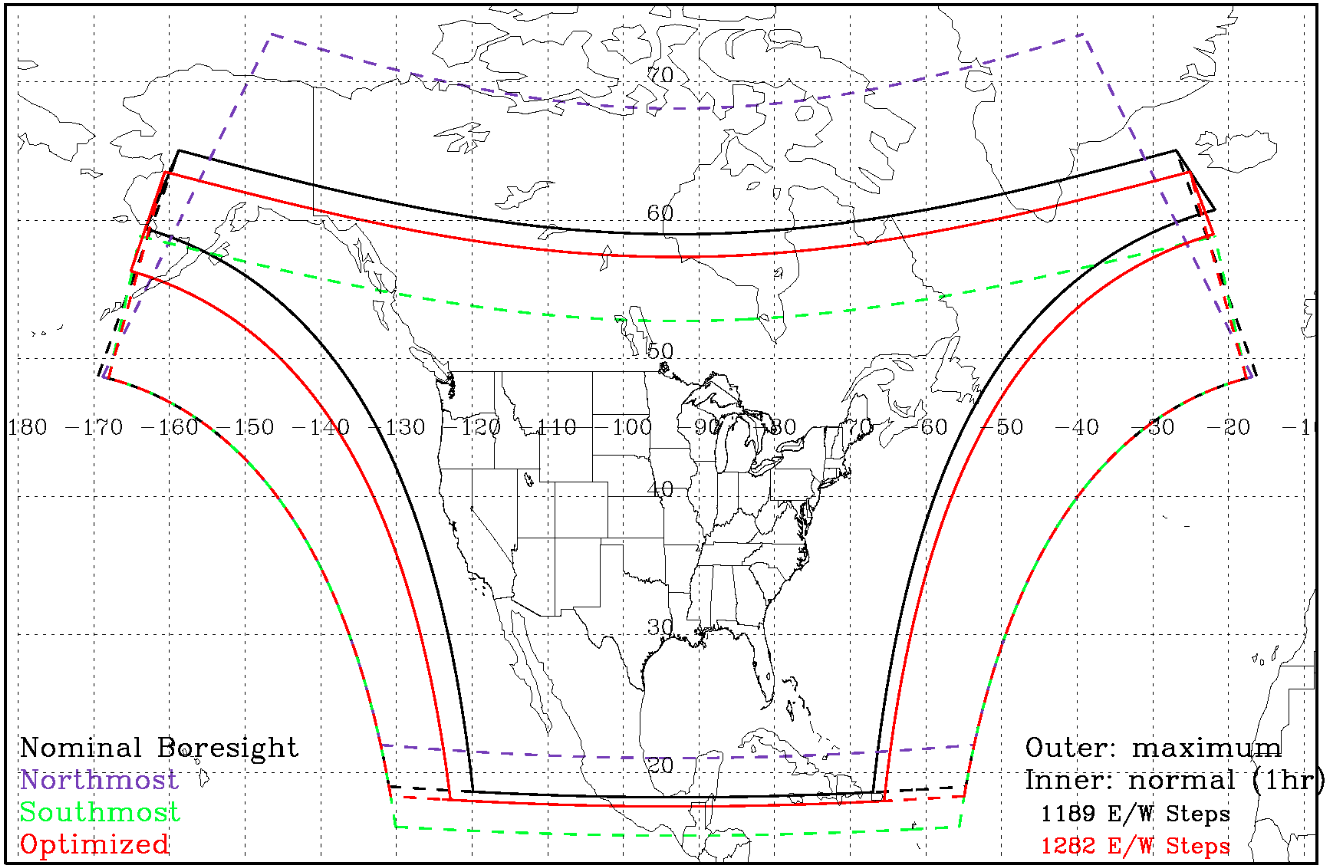
North-polar view
red=TEMPO FOR,
green=L3 boundary





L2 pixels, projected onto the Earth’s surface.
L3 pixel = blue square.

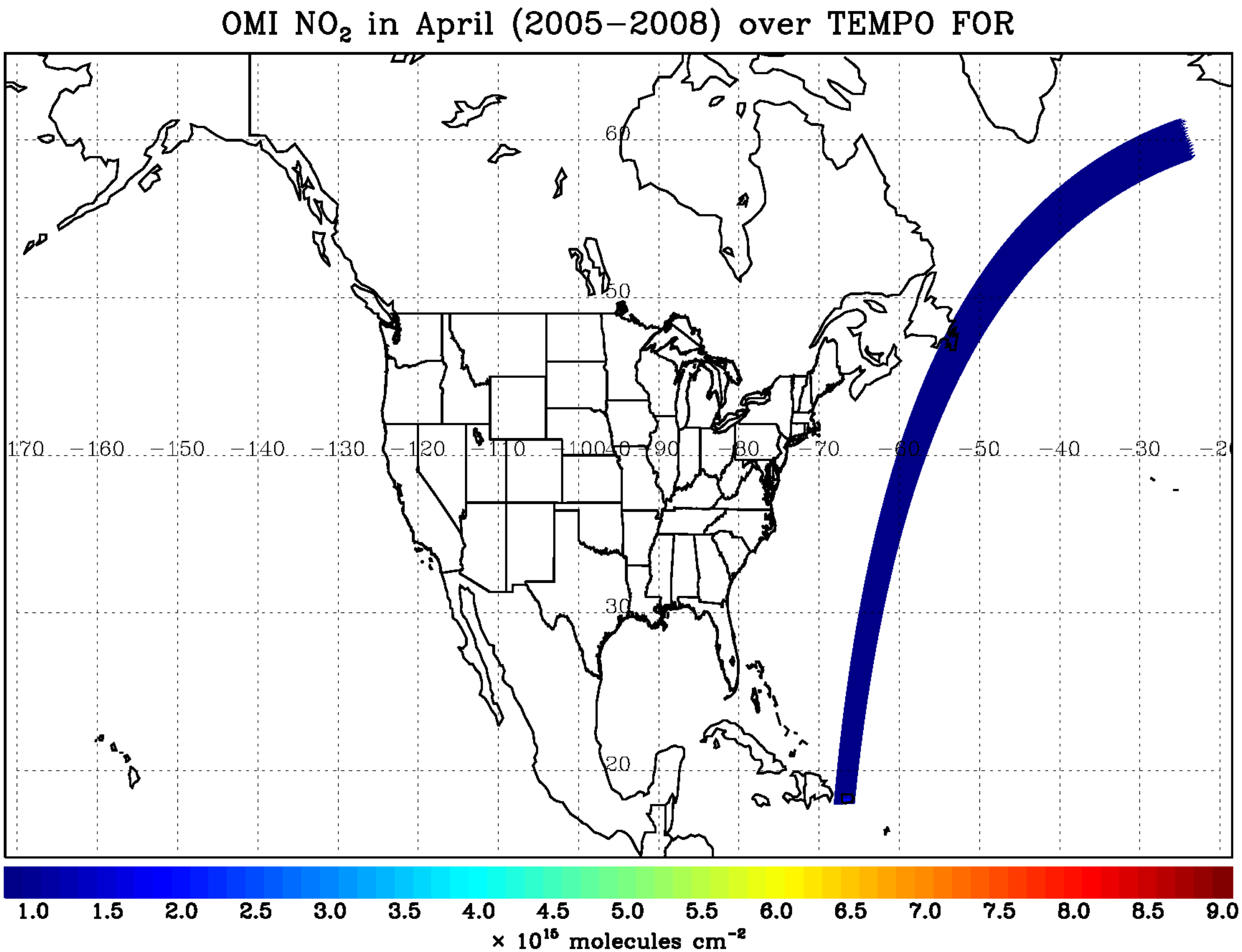
Expected performance



- 2035 good N/S pixels
- N/S IFOV: 41.49 μad
- E/W IFOV: 129.2 μad
- E/W step size: 123 μad (changeable, up to 200 μad)
- Allowable E/W range: 1614 steps
- Inner range of 1189 E/W steps: nominal boresight to cover CONUS in 1hr.
- Inner range of 1282 E/W steps: scan mirror @+950 μad S/N to cover Puerto Rico in 1 hr.

- Nominal boresight latitude: ~34.35ºN
- According to CONOPS document, scan mirror allowable range: ±4400 μad in dy or S/N, ± 49600 μrad in dx or E/W (x 2 for angle on ground)
- Maximum allowable E/W range for scan mirror between ± 49600 μrad E/W
- Northmost/Southmost range for scan mirror at -4400/+4400 μrad

TEMPO hourly NO_2 sweep (GEO @92.85W)



Boresight: 33.8°N, 93°W

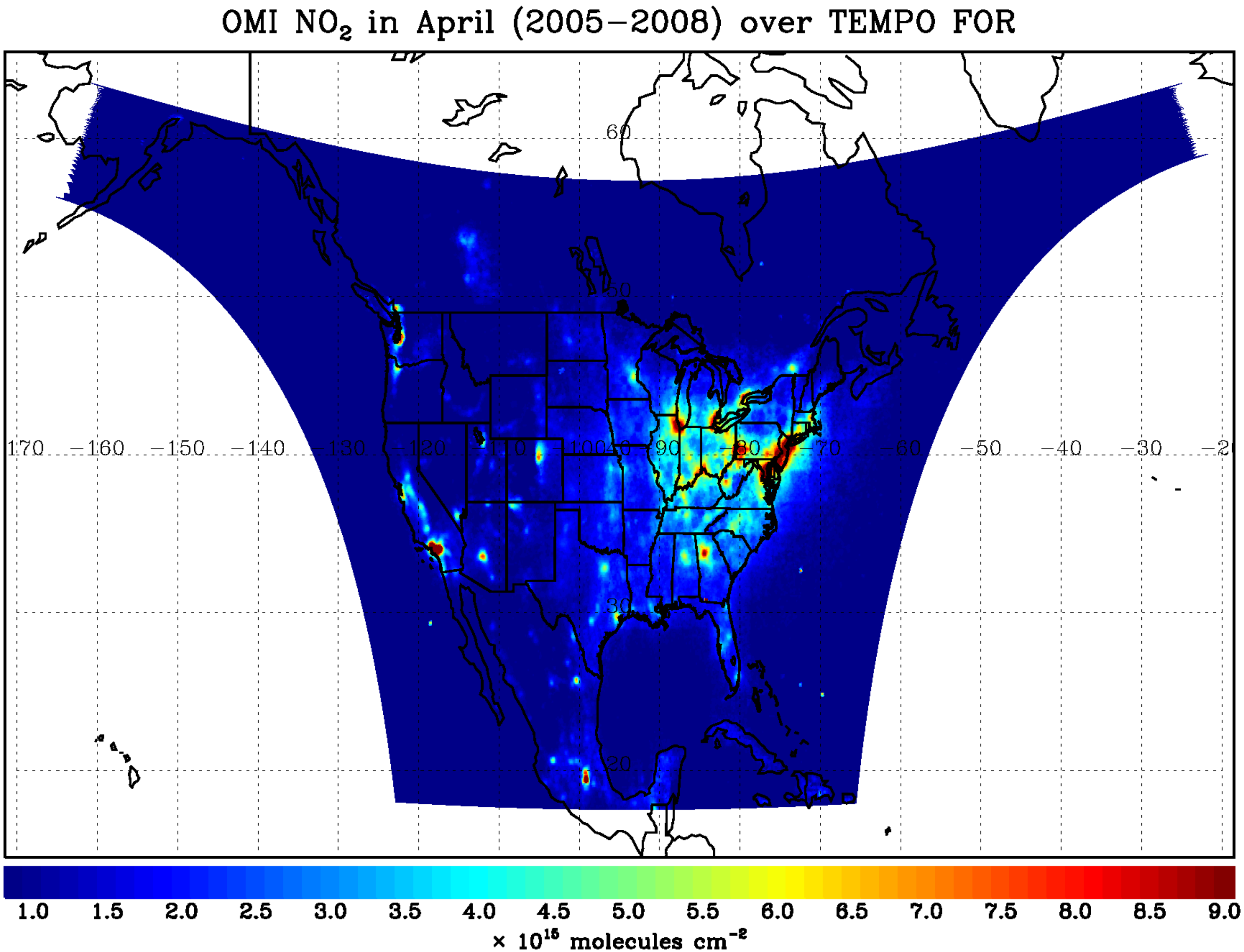
2034 good N/S pixels

- **~ 1282 scans/hr**
- **~ 2.6 M pixels/hr**

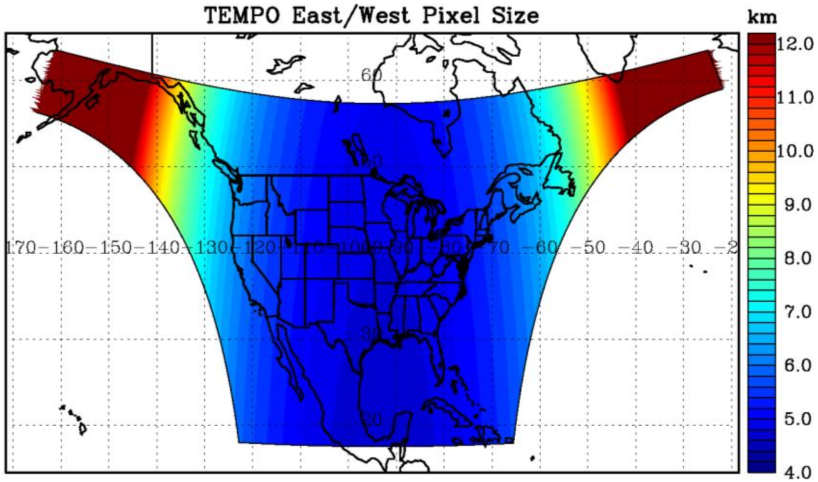
Data rate: ~31.2 Mbs

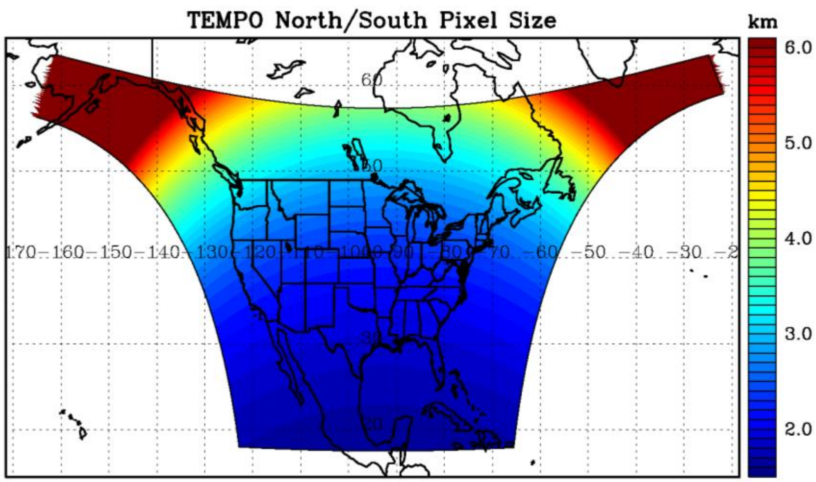
~20 times of OMI data volume (comparable to TROPOMI)

TEMPO hourly scan of NO_2 (GEO @92.85W)



TEMPO footprint (GEO @92.85° W)





- **Boresight at 33.76°N, 92.85°W**

Location	N/S (km)	E/W (km)	GSA (km^2)	VZA (°)
Boresight	2.0	4.8	9.5	39.3
36.5°N, 100°W	2.1	4.8	10.1	42.4
Washington, DC	2.3	5.1	11.3	48.0
Seattle	3.2	6.2	16.8	61.7
Los Angeles	2.1	5.6	11.3	48.0
Boston	2.5	5.5	13.0	53.7
Miami	1.8	4.9	8.6	33.2
San Juan	1.7	5.6	9.2	37.4
Mexico City	1.6	4.7	7.7	23.9
Can. tar sands	4.1	5.6	20.8	67.0
Juneau	6.1	9.1	33.3	75.3