Tropospheric Emissions: Monitoring of Pollution



TEMPO Products Overview

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Howelly Means

www.nasa.gov

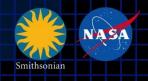
TEMPO

Outline



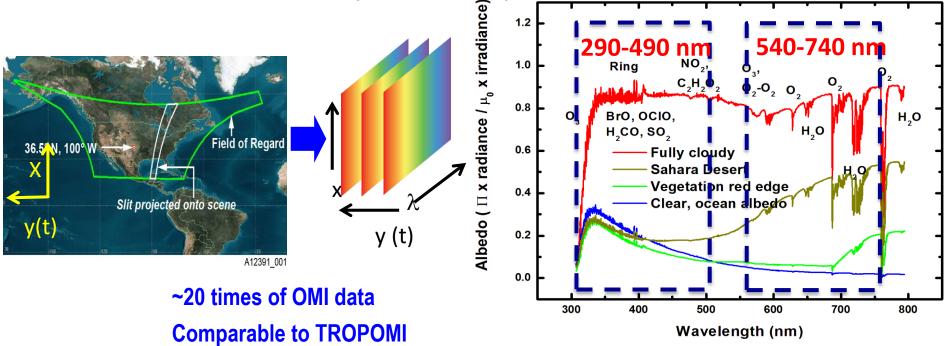
- ☐ Introduction
- Baseline products and research products
- Retrieval sensitivity studies, instrument performance and predicted retrieval performance
- Data products definitions (L0-L4) and details (e.g., format, data release, latency, archive, distribution)
- Overview of ground systems and science data processing center (SDPC)
- **Science algorithms (L0->L1, L1-L2, L2-L3, L2/3-L4)**

TEMPO



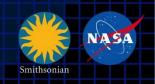
☐ Imaging grating spectrometer measuring solar backscattered Earth radiance

- > 0.6 nm FWHM, 0.2 nm sampling
- 290-490 + 540-740 nm, 2 channels (1 focal plane but with 2 2-D 2 k x 1k detectors)
- Geostationary, operating on commercial communication satellite as a hosted payload, with acceptable longitude range 115°W-80°W
 - **Great North America: Mexico City to Canadian tar sands, Atlantic to Pacific**
 - Instrument slit aligned N/S and sweep across the Field of Regard (FOR) in the E/W in 1 hour at ~2.1x4.5 km² (center of FOR) with ~2.6M spatial pixels/hr





Baseline and threshold data products



Species/Products	Required Precision	Temporal Revisit	Aerosols (AOD, SSA,
0-2 km O ₃ (Selected Scenes) Baseline only	10 ppbv	2 hour	AAI), SO ₂ , C ₂ H ₂ O ₂ were removed from baseline
Tropospheric O ₃	10 ppbv	1 hour	products during KDPC
Total O ₃	3%	1 hour	Use reserve to bring them back during gap period
Tropospheric NO ₂	1.0×10^{15} molecules cm ⁻²	1 hour	back during gap period
Tropospheric H ₂ CO	1.0×10^{16} molecules cm ⁻²	3 hour	Cloud product (cloud
Tropospheric SO ₂	1.0 × 10 ¹⁶ molecules cm ⁻²	3 hour	fraction, cloud pressure):
Tropospheric C ₂ H ₂ O ₂	4.0×10^{14} molecules cm ⁻²	3 hour	used in trace gas retrievals
Aerosol Optical Depth	0.10	1 hour	

- Minimal set of products sufficient for constraining air quality
- Across GNA: 18°N to 58°N near 100°W, 67°W to 125°W near 42°N
- Data products at urban-regional spatial scales
 - Baseline ≤ 60 km² at center of Field Of Regard (FOR)
 - Threshold \leq 300 km² at center of FOR
- Temporal scales to resolve diurnal changes in pollutant distributions
- Geolocation uncertainty of less than 4 km
- Mission duration, subject to instrument availability
 - Baseline 20 months
 - Threshold 12 months

TEMPO TEMPO Launch Algorithms for Standard Products



NO₂, H₂CO, SO₂, C₂H₂O₂ vertical columns

Direct fitting to TEMPO radiances (e.g., OMHCHO) AMF-corrected reference spectra, Ring effect, etc. NO_2 strat/trop separation (STS) adapted from OMI Research products could include H₂O, BrO, OCIO, IO

O₃ profiles and tropospheric O₃

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

Cloud Products from OMCLDRR: CF, CTP

Advanced/improved products likely developed at GSFC

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

Other Research Products

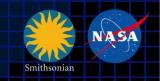
- TEMPO research products will greatly extend science and applications
 - H₂O, BrO, OCIO, IO, volcanic (SO₂ plume height and VCD), and more species (e.g., HONO?)
 - > Additional/improved cloud with $O_2 O_2$ bands or $O_2 B$ bands
 - Additional aerosol products from hyperspectral spectra, O₂-B and O₂-O₂-bands, and TEMPO + GOES-R synergy at @U lowa, GSFC, NOAA
 - Vegetation products: solar Induced fluorescence (SIF)
 - Diurnal out-going shortwave radiation and cloud forcing
 - City lights

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Higher-level products: Near-real-time pollution/AQ indices, UVB/UV index



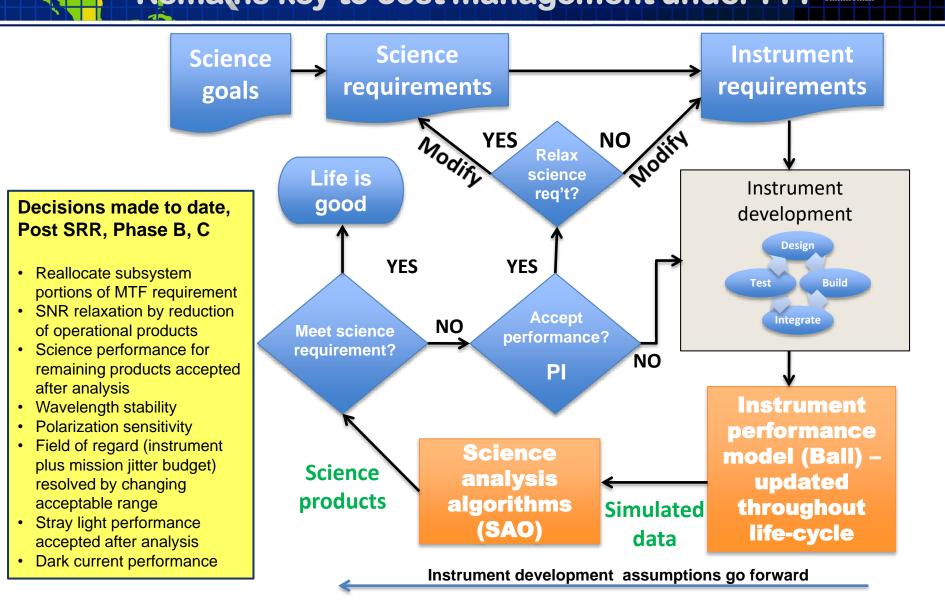
TEMPO Retrieval Sensitivity Studies



- 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 (O₃, NO₂, H₂CO, SO₂, C₂H₂O₂, H₂O), BrO, OCIO, O₂, O₄' 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 O₃, unconstrained for other trace gas VCDs, consistent with current algorithms
 - > Optimal estimation to perform retrieval sensitivity and error analysis

Remains key to cost management under FFP

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TEMPO Instrument 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 Volume		$\begin{array}{l} 148 \text{ kg} \\ 1.4 \times 1.1 \times 1.2 \text{ m} \end{array}$	Spectral range Spectral resolution & sampling	290–490 nm, 540–740 nm 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]	O₃: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
Zoogman et al.,	H ₂ CO: 327–356 nm	2503	Field of regard: N/ $S \times E/W$	$4.82^{\circ} \times 8.38^{\circ}$ (greater North America)
200gman et al.,	SO ₂ : 305–345 nm	1797	Geo-location Uncertainty	2.8 km
2017, JQSRT,	C ₂ H ₂ O ₂ : 420– 480 nm	1679	IFOV: $N/S \times E/W$	2.1 km × 4.4 km
TEMPO Overview	Aerosol: 354, 388 nm	2313	E/W oversampling	5%
	Clouds: 346– 354 nm	2492	MTF of IFOV: N/S $\times E/W$	0.19 imes 0.36

* SNR are for 4 pixels coadded as requirements are derived from coadding 4 pixels at 8.4 x 4.5 km²!



TEMPO Retrieval Performance



Table 3.

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

UV total O_3 0.32 ± 0.08 0.72 ± 0.08 100 > O_3 : fitting precisionUV trop. O_3 3.05 ± 0.71 6.38 ± 1.98 98.3vertical smoothing,	Product ^a	Precision	Total errors	Meets reqs. (%)	Clear-sky conditions
UV/Vis total O_3 0.30 ± 0.07 0.54 ± 0.13 99.4 > Other trace gases:UV/Vis trop. O_3 3.04 ± 0.90 5.21 ± 1.72 98.9 > Other trace gases:UV/Vis $0-2 \text{ km } O_3$ 3.29 ± 0.71 7.93 ± 1.41 92.8 fitting precision,NO_2 (× 10^{15}) 0.30 ± 0.08 0.36 ± 0.20 98.4 interference.	UV trop. O_3 UV 0-2 km O_3 UV/Vis total O_3 UV/Vis trop. O_3 UV/Vis 0-2 km O_3 NO ₂ (× 10 ¹⁵) H ₂ CO (× 10 ¹⁶) C ₂ H ₂ O ₂ (× 10 ¹⁴)	$\begin{array}{c}$	6.38 ± 1.98 8.86 ± 1.53 0.54 ± 0.13 5.21 ± 1.72 7.93 ± 1.41 0.36 ± 0.20 0.42 ± 0.13 4.75 ± 1.62	100 >> 98.3 78.2 99.4 98.9 92.8 98.4 100 N/A	O ₃ : fitting precision, vertical smoothing, interferences Other trace gases: fitting precision, interference. Uncertainties due to profile shape not

Zoogman et al., 2017, JQSRT, TEMPO Overview

^a The units are % for total ozone column, ppbv for tropospheric O_3 and O_2 km O_3 , and molecules cm⁻² for other trace gases.



Data Products (L1-L4) Definitions and Details



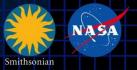
Data Product	Description	Time beyond on- orbit checkout to deliver initial data	Maximum data latency after first release for ≥ 80% of all products [†]
Level 0	Reconstructed, Unprocessed Instrument Data	2 months	Within 2 hours of receipt at SAO
Level 1b	Calibrated, Geolocated Radiances	4 months	Within 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, mostly within 3 hours except for O ₃ profile
Level 3	Derived Gridded Geophysical Data Products (daily, monthly)	6 months	1 month after completion of data accumulation required for individual geophysical products
Level 4	Derived from multiple Level 2-3 products (e.g., AQ index, UV index)	Not operational, pr	roduced on best effort basis

Data products are generated in NetCDF4/HDF5 format with basic ODL-format metadata (can be converted to XML at ASDC)

All original observation & standard science data products shall be delivered to NASA LaRc ASDC at within 6 months of completion of the prime mission (plan to archive it as soon as it's generated). Data products are publicly distributed during the mission. ⁺80% of the products, not 80% of the product types, will be produced within this latency time. 11

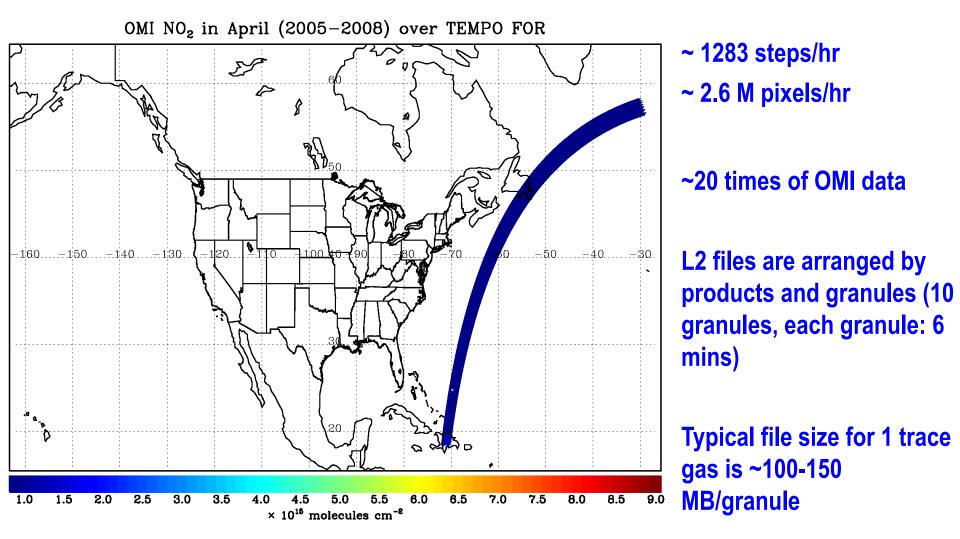
4PO List of Specific Data Products

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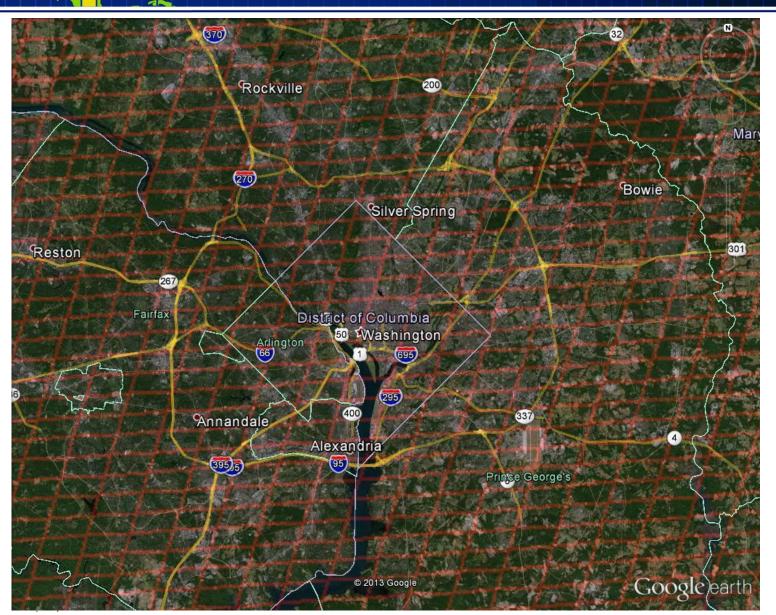
Level	Product	Algorithm	Major Outputs	Spa Res km ²	Freq/Size
L1-b	irradiance	SAO LO-1	Calibrated & quality flags		daily
	radiance	SAO L0-1	Geolocated,calibrated, viewing,geolocation& quality flags	2.1 x 4.5	Hourly, granule
L2	Cloud	OMCLDRR	Cloud fraction, cloud pressure	2.1 x 4.5	Hourly, granule
	O3 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 O3	TOMS V8.5	Total O3, AI, cloud frac	2.1 x 4.5	Hourly, granule
	NO2	SAO trace gas Dalhousie/BU strat/trop sep.	SCD, strat./trop. VCD, error, shape factor, scattering weights	2.1 x 4.5	Hourly, granule
	H2CO	SAO trace gas		2.1 x 4.5	Hourly, granule
	SO2	SAO trace gas	SCD, VCD, error, shape factor,	2.1 x 4.5	Hourly, granule
	C2H2O2	SAO trace gas	SCD, VCD, error, shape factor, scattering weights	2.1 x 4.5	Hourly, granule
	H2O,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	Dalhousie, EPA	Air quality index	TBD	Hourly, scan
	UVB	OM UVB	UV irradiance, erythemal irradiance, UV index	TBD	Hourly, scan

TEMPO hourly NO₂ sweep



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Washington, DC coverage



100

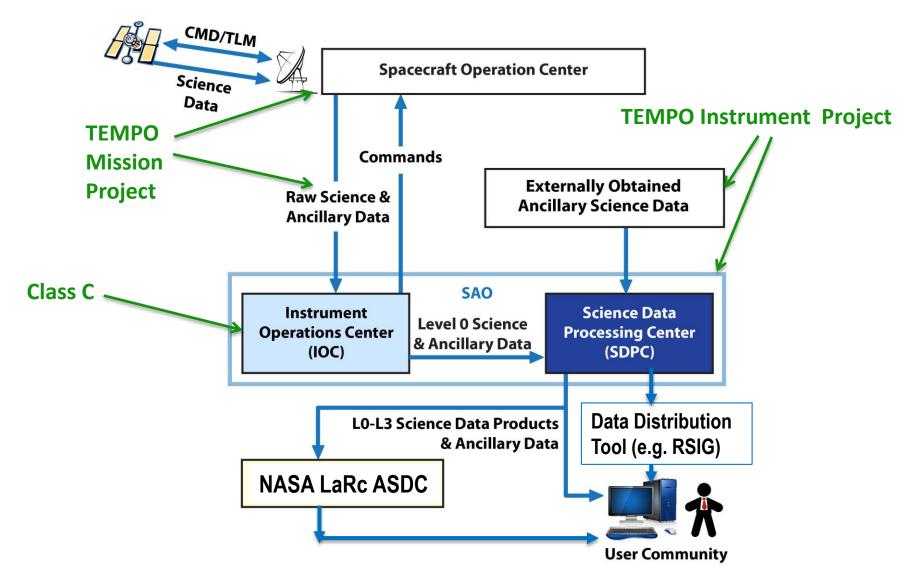
Geolocations will be provided at 4 corners and pixel center

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Ground Systems Overview

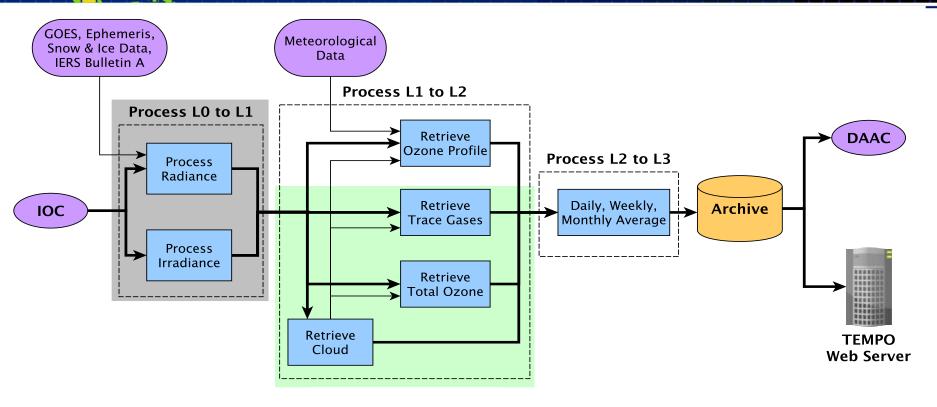
NPO



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Science Data Processing **Center (SDPC) Overview**



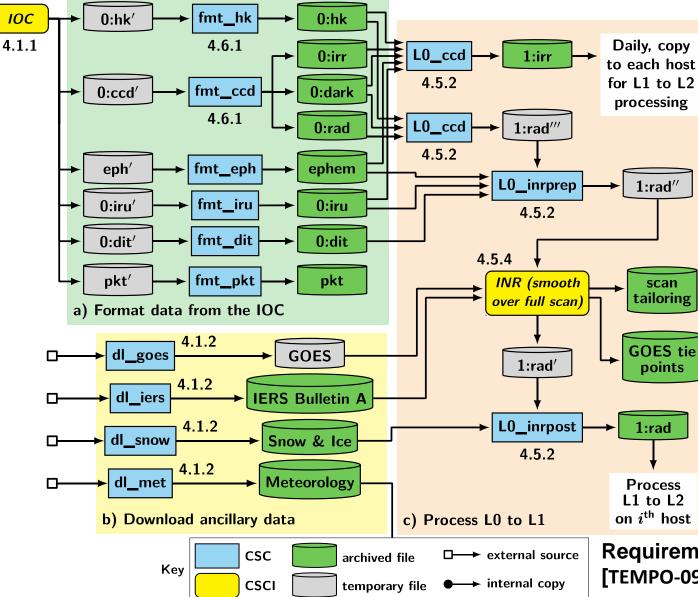
- L0-L1 algorithm is developed at SAO.
- \succ L1/L2: netCDF4/HDF-5.
- L1->L2: Cloud, total ozone, trace gas code, ozone profile, aerosols.
- L2->L3: re-gridding of L2 products to standard longitude-latitude grid cells hourly at daily/weekly/monthly scales 16

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L0-1 Processor



Heritages from:
 OMI, TROPOMI,
 OMPS,
 GOME/GOME-2,
 GEOTASO

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 TEMPO specifics
 INR (geo-location) by Carr Astronautics
 T-dependent dark current correction
 Polarization correction

Requirements from SDPCRD [TEMPO-09-0003] labeled as 4.X.X

TEMPO Cloud Algorithm



Adapted from OMCLDRR to retrieve <u>effective cloud fraction</u> and optical centroid pressure (OCP) from TEMPO normalized radiances in ~346-354 nm

- Rotational Raman Scattering (RRS) cloud algorithm developed for OMI titled 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 lookup table

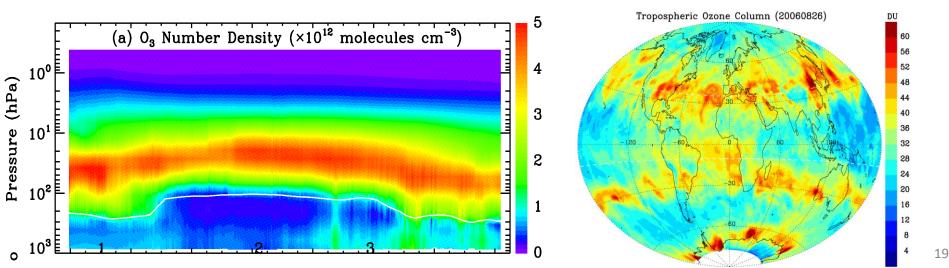
The RRS cloud retrievals are sensitive to instrumental (e.g., stray light, dark current), geophysical effects (e.g., 3D, shadow)

Backup algorithm is being developed based on absorption O2-O2 at 477 nm at GSFC 18

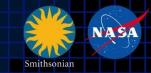
TEMPO Ozone Profile and Tropospheric O₃ Algorithm



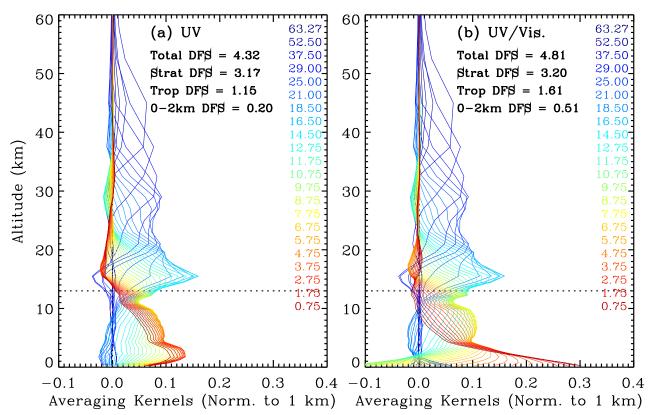
- Adapted SAO OE-based algorithm developed for GOME and OMI (Liu et al., 2005, 2010) to retrieve partial ozone columns at ~24 layers as well as total, stratospheric, tropospheric, and 0-2 km ozone columns from normalized radiance in the UV (290-345 nm) and visible (540-650 nm)
 - Climatological a priori: tropopause-based O₃ profile climatology (Bak et al., 2013) or diurnally resolved O₃ 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



TEMPO TEMPO Ozone Profile and Tropospheric O₃ Algorithm



- 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 km², data latency within 24 hours

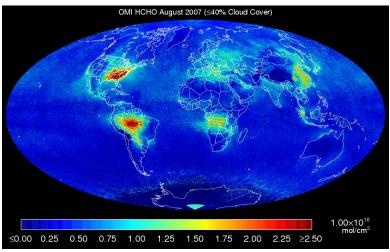


TEMPO Trace Gas Algorithm

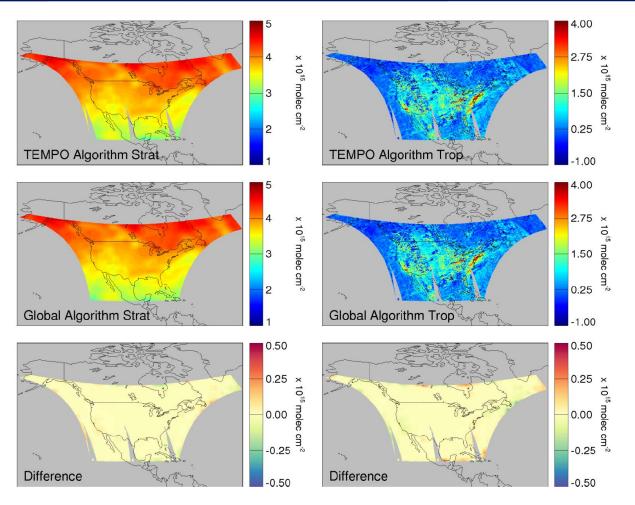
Adapted from SAO two-step OMI trace gas algorithm and NASA NO₂ stratospheric/tropospheric separation (STS) algorithm to retrieve VCDs of trace gases (e.g., NO₂, H₂CO, SO₂, C₂H₂O₂) from

- 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





TEMPO TEMPO NO2 Strat./Trop. Separation (STS) Algorithm



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J. Geddes (BU) and R. Martin (Dalhousie Univ.) adapted NASA OMI NO₂ STS algorithm to TEMPO (limited domain) and found small errors of ~2.0E14 molecules at the edge. 22

TEMPO Aerosol and Total Ozone Algorithms

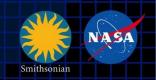


- Will adapt from OMAERUV developed by O. Torres at GSFC to retrieve <u>Absorbing Aerosol Index (AAI)</u>, <u>Aerosol Optical Depth</u> (AOD), and <u>Single Scattering Albedo (SSA)</u> from TEMPO normalized radiances at ~354 and 388 nm.
 - Uses the sensitivity of near-UV observations to particle absorption 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 CALIPO (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 km².

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)



Hourly Level 3 product is a re-gridding of Level 2



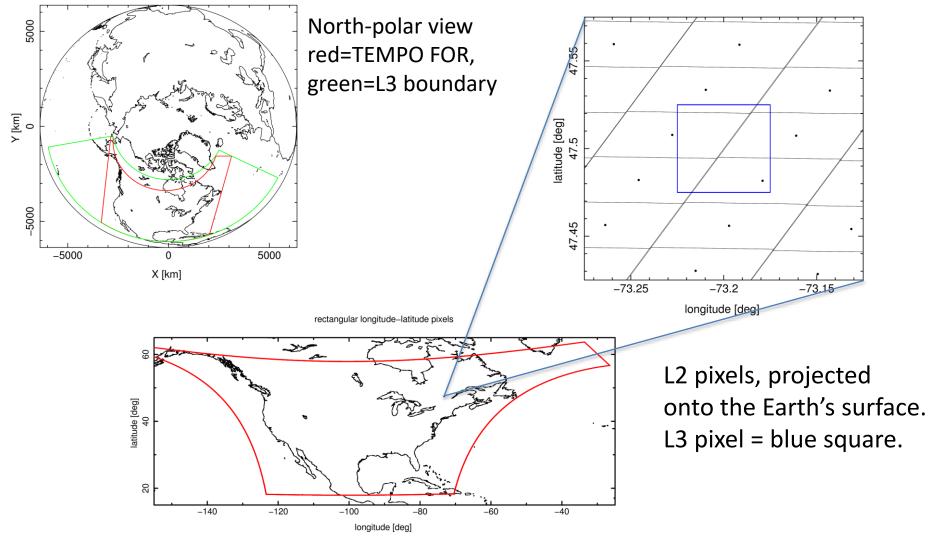
- > L2 products are trace gas column densities plus related variables
 - derived per-granule, with minimal spatial overlap
 - defined in projection onto a virtual detector plane (individual TEMPO pixels)
- L3 product involves re-gridding selected L2 product variables onto a longitude-latitude grid with square pixels.
 - Each L3 pixel value is an area-weighted (and also uncertaintyweighted) 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.



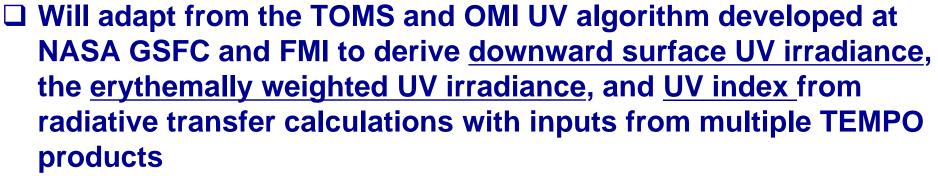
Re-gridding of Level 2 data products

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pix = 0.05 deg @ -73.2W, +47.5N



TEMPO UVB Algorithm



- Total ozone, scene reflectance at ~360 nm
- Cloud product
- Surface albedo climatology
- Aerosol product or aerosol climatology

TEMPO Air Quality and Health

TEMPO's hourly measurements allow better understanding of the complex chemistry and dynamics that drive air quality on short timescales. The density of TEMPO data is ideally suited for data assimilation into chemical models for both air quality forecasting and for better constraints on emissions that lead to air quality exceedances. Planning is underway to combine TEMPO with regional air quality models to improve EPA air quality indices and to directly supply the public with near real time pollution reports and forecasts through website and mobile applications. As a case study, an OSSE for the Intermountain West was performed to explore the potential of geostationary ozone measurements from TEMPO to improve monitoring of ozone exceedances and the role of background ozone in causing these exceedances (Zoogman et al. 2014).



AQ Indices



What is an AQ index?"

"The Canadian Air Quality Health Index is a multipollutant index based on the sum of PM2.5, NO_2 , and O_3 , weighted by their contribution to mortality in daily time-series study across Canadian cities." [Cooper et al., 2012]

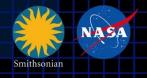
Cooper et al., for example, propose a satellite-based multipollutant index using the WHO Air Quality Guidelines (AQG):

$$SATMPI = \frac{PM_{2.5}}{AQG_{PM2.5}} \left[1 + \frac{NO_2}{AQG_{NO_2}} \right]$$

- Can we define different indices as appropriate to locations, seasons, times?
- Might they be formulated using RSIG?
- Might assimilation be included?

Cooper, M., R.V. Martin, A. van Donkelaar, L. Lamsal, M. Brauer, and J. Brook, A satellite-based multi-pollutant index of global air quality, *Env. Sci. and Tech.*, **46**, 8523-8524, 2012.





TEMPO will provide hourly atmospheric pollution at high spatial resolution (~10 km² at center of FOR) over North America from the GEO orbit.

TEMPO data products and science algorithms are briefly reviewed.



Journal of Quantitative Spectroscopy & Radiative Transfer

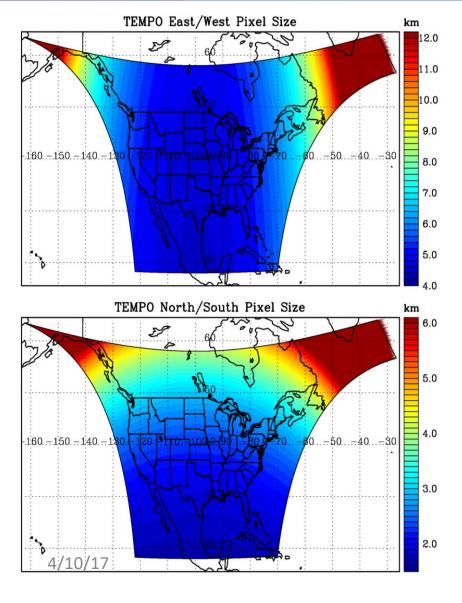
journal homepage: www.elsevier.com/locate/jqsrt

Tropospheric emissions: Monitoring of pollution (TEMPO)

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TEMPO footprint (GEO at 100° W)



Location	N/S (km)	E/W (km)	GSA (km²)
36.5°N, 100°W	2.11	4.65	9.8
Washington, DC	2.37	5.36	11.9
Seattle	2.99	5.46	14.9
Los Angeles	2.09	5.04	10.2
Boston	2.71	5.90	14.1
Miami	1.83	5.04	9.0
Mexico City	1.65	4.54	7.5
Canadian oil sands	3.94	5.05	19.2

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Assumes 2000 N/S pixels

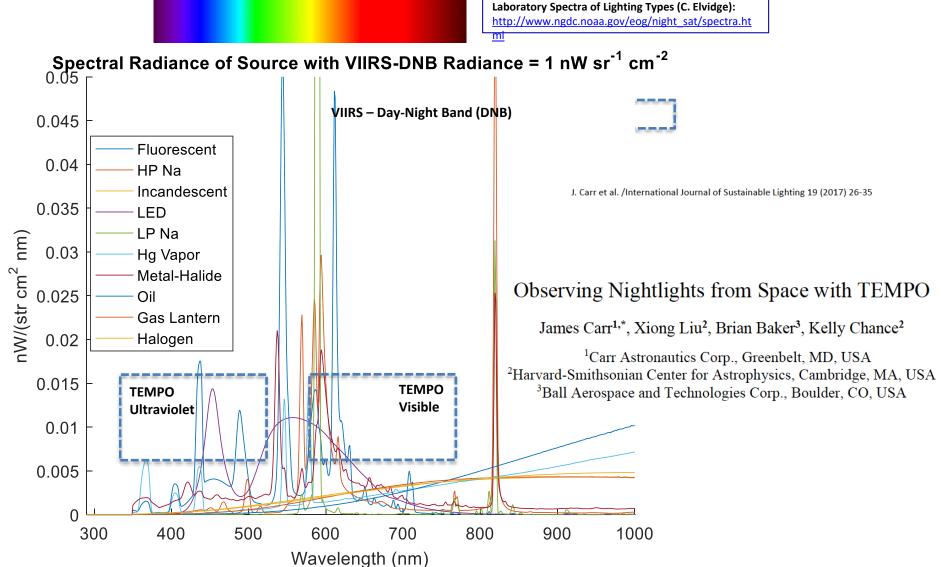
For GEO at 80°W, pixel size at 36.5°N, 100°W is 2.2 km \times 5.2³¹ km.



Nighttime city lights products, which represent anthropogenic activities at the same spatial resolution as air quality products, may be produced twice per day (late evening and early morning) as a research product. Meeting TEMPO measurement requirements for NO_2 (visible) implies the sensitivity for city lights products over the CONUS within a 2-hour period at 2×4.5 km² to 1.1×10^{-8} W cm⁻² sr⁻¹ µm⁻¹.

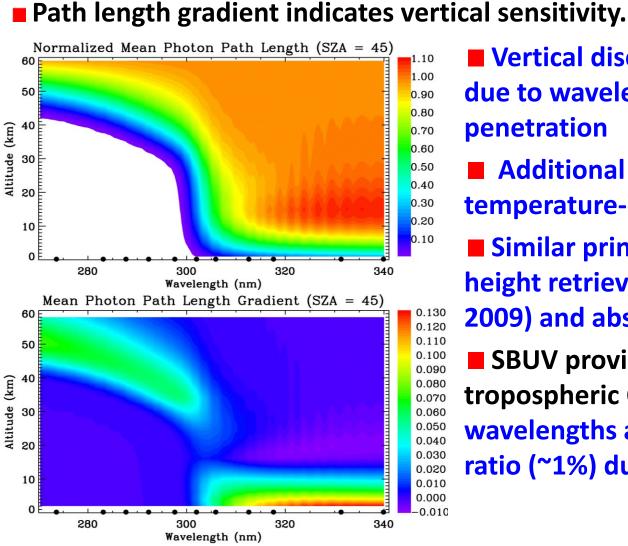
City lights

Night Lights Spectroscopic Signatures



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Physical principles of BUV Ozone Profile Retrievals (1996), Chance et al. (1997) Normalized photon path length: 0: no photo penetration, <1, not all photons penetrate to that level, >1, enhancement due to multiple scattering



Vertical discrimination is primarily due to wavelength-dependent photon penetration

■ Additional tropospheric O₃ info. from temperature-dependent Huggins bands

 Similar principle applies to plume height retrievals of SO₂ (Yang et al., 2009) and absorbing aerosols

■ SBUV provides little vertical tropospheric O₃ information: too few wavelengths and poor signal to noise ratio (~1%) due to spatial aliasing

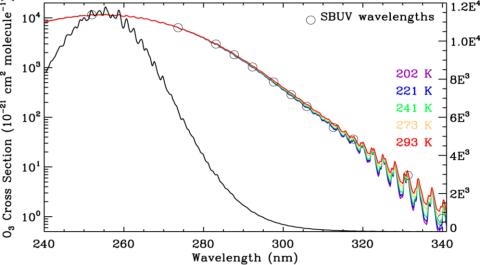
TEMPRV sical Principles of BUV Ozone Profile Retrievals

udy by chance et al. (1996, JQSRT): Possible

SATELLITE MEASUREMENTS OF ATMOSPHERIC OZONE PROFILES, INCLUDING TROPOSPHERIC OZONE, FROM ULTRAVIOLET/VISIBLE MEASUREMENTS IN THE NADIR GEOMETRY: A POTENTIAL METHOD TO RETRIEVE TROPOSPHERIC OZONE

backscattered UV and visible spectra

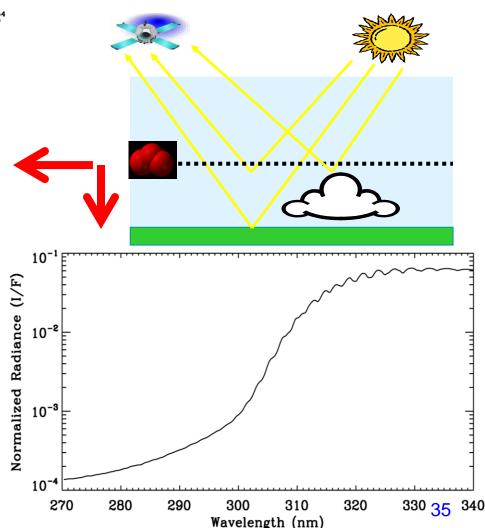
K. V. CHANCE, ^e J. P. BURROWS, ^b D. PERNER, ^c and W. SCHNEIDER^d "Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, U.S.A., ^hInstitute of Remote Sensing, University of Bremen, Bremen, Germany, 'Atmospheric Chemistry Division, Max Planck Institute for Chemistry, Mainz, Germany, and 'Euromap GmbH, Neustrelitz, Germany



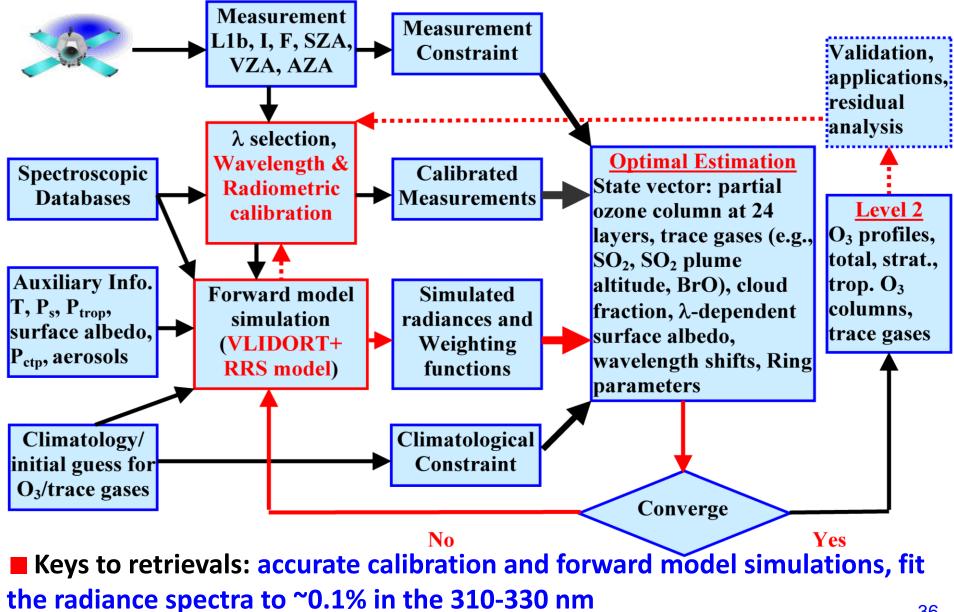
Several important implications that makes retrievals challenging:

4 Radiances are often measured in several channels

Subject to wavelength and radiometric calibration errors especially at shorter wavelengths, offset between various channels



O OMI Ozone Profile Retrieval Algorithm NASA

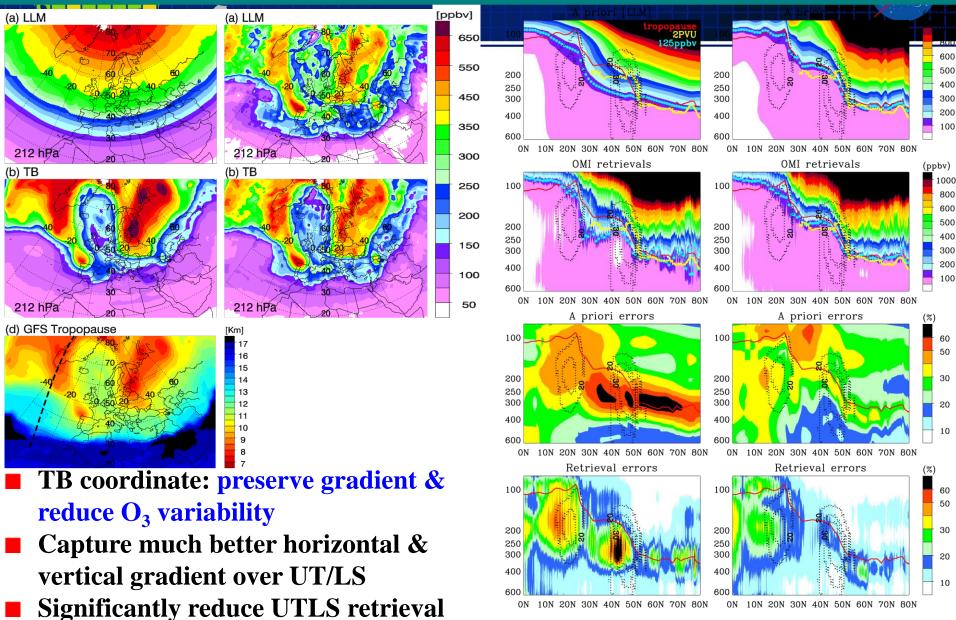


EMPO

The Use of Tropospause-based Climatology

errors





ON 10N 20N 30N 40N 50N 60N 70N 80N

ON 10N 20N 30N 40N 50N 60N 70N 80N

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