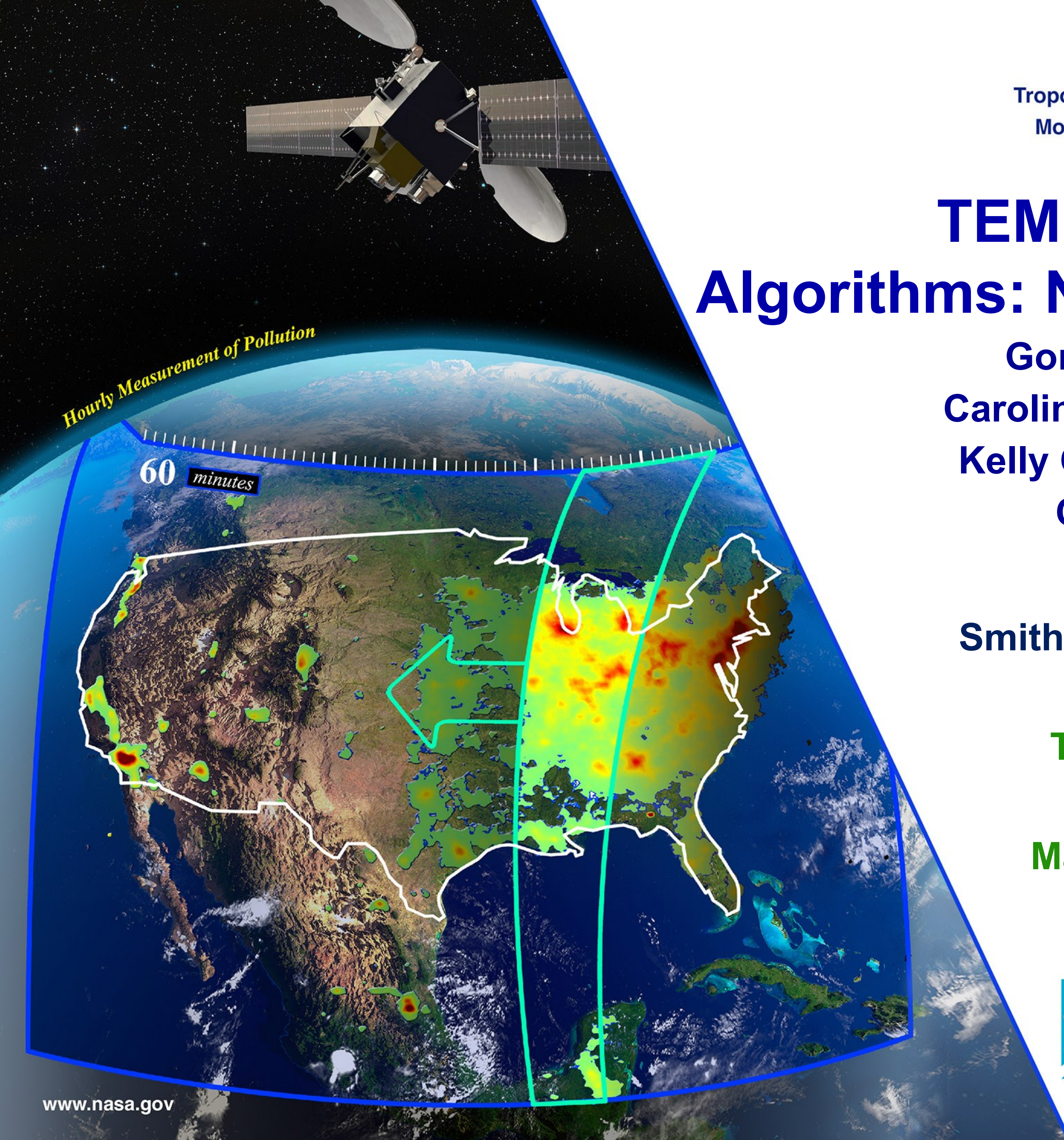

Tropospheric Emissions:
Monitoring of Pollution

TEMPO Trace Gas Algorithms: NO_2 and H_2CO

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Chris Chan Miller and
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Smithsonian Astrophysical Observatory

TEMPO Science Team Meeting 2022

May 31 – June 02, 2022

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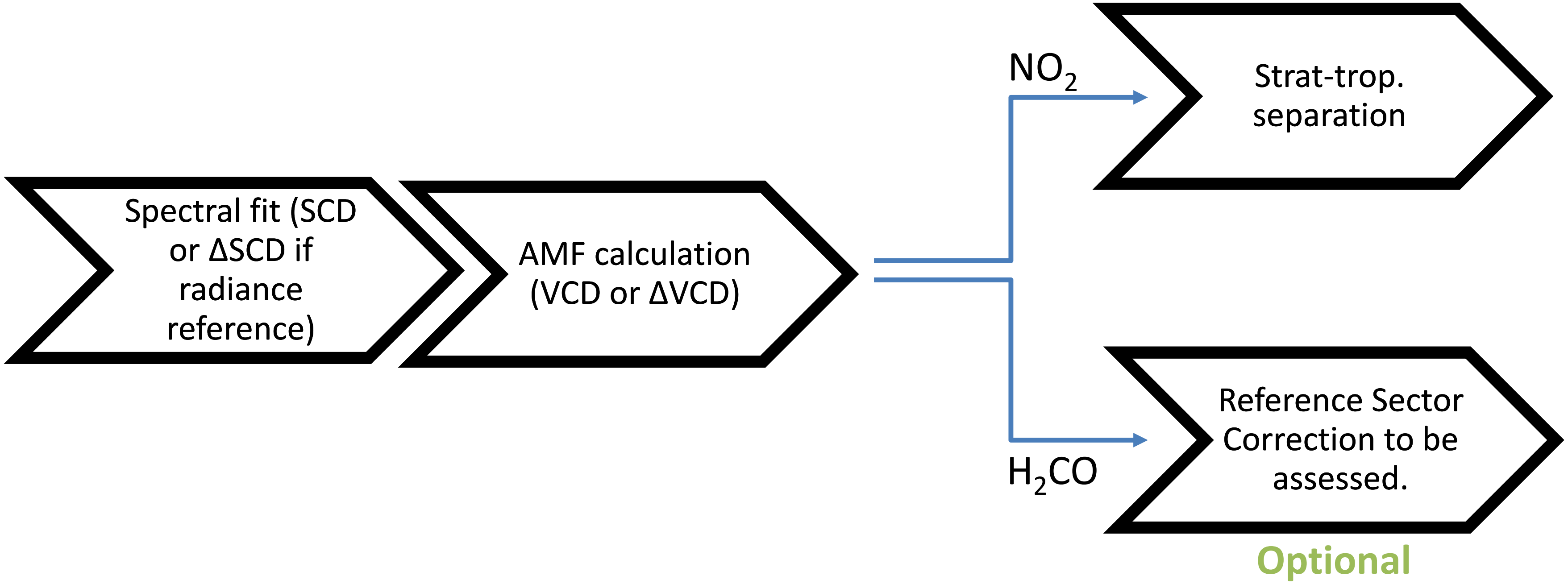
Trace gas algorithm approach

Three major steps constitute the NO_2 and H_2CO retrievals. Common steps to both algorithms are the spectral fit (retrieval of SCDs) and calculation of Air Mass Factors.



A third step for NO_2 includes the stratospheric/tropospheric separation and in the case of H_2CO optional corrections associated with the use of radiance reference or striping.

Spectral fit: direct fit of radiances

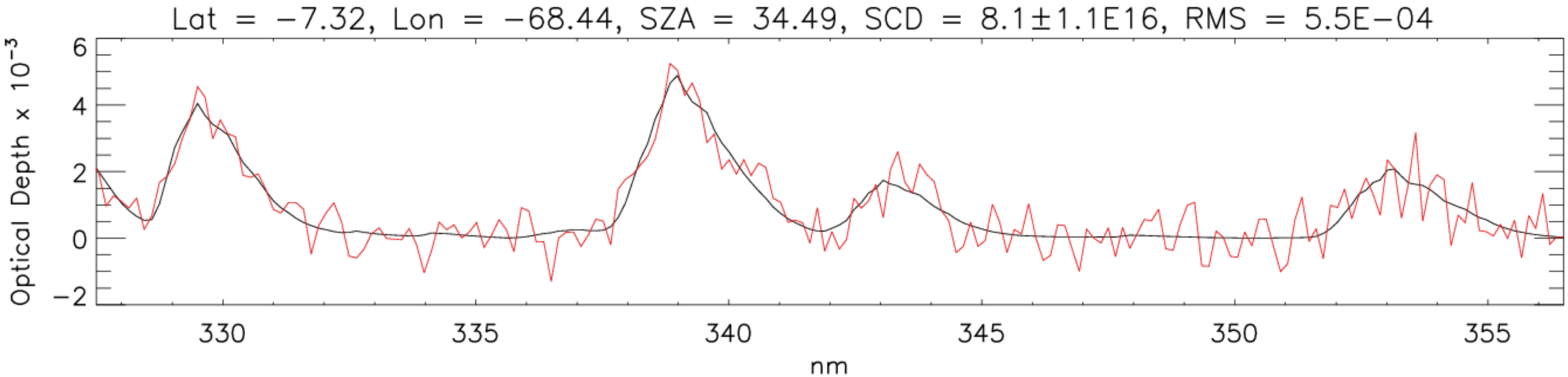
Read L1 data → Read auxiliary data

Wavelength calibration using high resolution solar spectrum (optional is the fitting of slit functions using super-Gaussian parameterization)

Compute I0 corrections, under-sampling corrections, common mode to represent systematic residuals (optional)

Direct fitting of slant columns

$$I = \left[\left(aI_o + \sum_i \alpha_i X_i\right) e^{-\sum_j \alpha_j X_j} + \sum_k \alpha_k X_k \right] ScalPoly + BasePoly$$

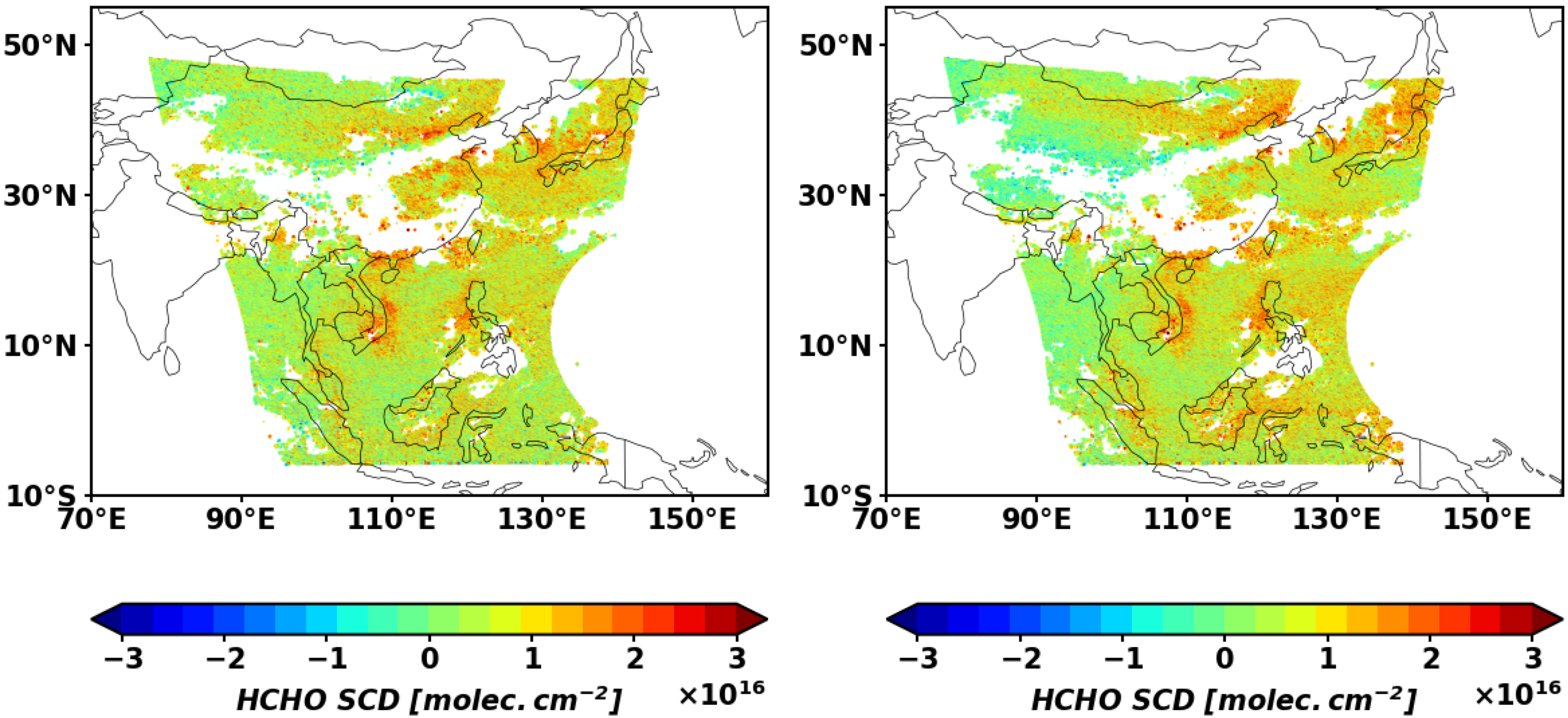


NO_2 and H_2CO spectral fit set up

Parameter	NO_2	H_2CO
Fitting window	405 - 465 nm	328.5 - 356.5 nm
Baseline polynomial	3^{rd} order	3^{rd} order
Scaling polynomial	4^{th} order	3^{rd} order
Solar reference spectrum	Chance and Kurucz (2010)	
Raman Scattering	Derived using Chance and Spurr (1997)	
Undersampling correction	Derived using Chance et al. (2005)	
Reference cross sections	•O_3 Serdyuchenko et al. (2014) at 223K •NO_2 Vandaele et al. (1998) 220K •O_2-O_2 Thalman and Volkamer (2013) at 293 K. May update to Finkenzeller and Volkamer (2022). •H_2O HITRAN 2020 at 293K •Liquid H_2O Mason and Fry (2016)	•O_3 Serdyuchenko et al. (2014) at 223K and 243K •NO_2 Vandaele et al. (1998) 220K •O_2-O_2 Thalman and Volkamer (2013) 293 K. May update to Finkenzeller and Volkamer (2022). •BrO Wilmouth et al. (1999) 228K •H_2CO Chance and Orphal (2011) 300K

H_2CO spectral fit example using GEMS data

GEMS algorithm **20210601 0045 UTC** **TEMPO**



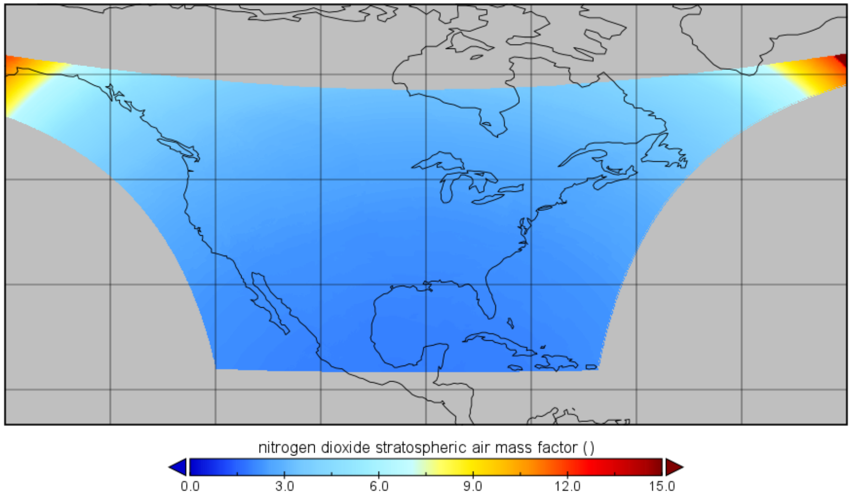
In this particular example, both GEMS and TEMPO, use radiance reference as source term in the modelled spectrum

AMF calculation

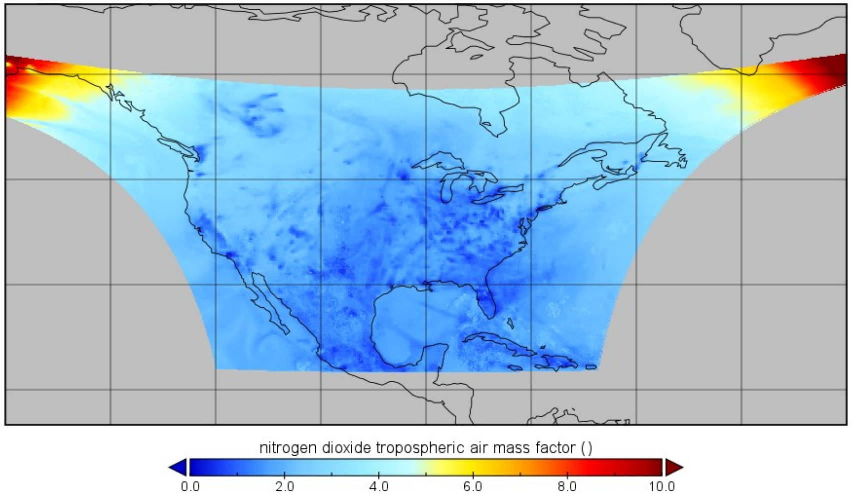
Input	Source
Cloud fraction and pressure	TEMPO cloud product. Defaults to a cloud pressure climatology (OMI-derived) if cloud retrieval is unavailable.
Trace gas profiles	GEOS-CF hourly forecast from prior day (25-km resolution). Defaults to monthly 1-hour climatology derived from GEOS-CF if forecast is unavailable.
Vertical layers	72 layers on GEOS-CF vertical grid
Surface albedo	GLER climatology from OMI GSFC team (0.05° resolution) Over land (Fasnacht et al., 2019): derived from MODIS BRDF, extended to shorter wavelengths 340 nm (H_2CO) and 440 nm (NO_2) using visible surface reflectance EOFs updated from Zoogman et al. (2016) and SCIAMACHY reflectance climatologies. Over water (Qin et al., 2019): derived using surface wind speed
Snow/ice fraction	IMS snow and ice (1-km resolution)
Meteorological variables: Temperature profile (for hypsometric equation and NO_2 T-dependency), surface pressure, tropopause pressure (for NO_2 stratospheric correction), wind speed (for ocean GLER)	GEOS-CF hourly forecast from prior day (25-km resolution). Defaults to monthly 1-hour climatology derived from GEOS-CF if forecast is unavailable.
Terrain height correction	Corrected following Boersma et al. (2011) using GMTED2010 (30 arcsec) DEM
Aerosols	Not applied (considered implicitly in cloud retrieval)

AMF calculation example

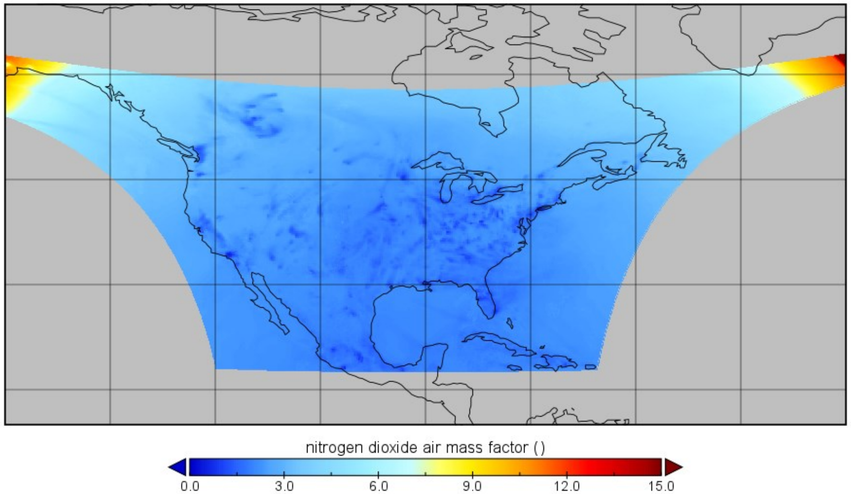
NO$_2$ stratospheric AMF



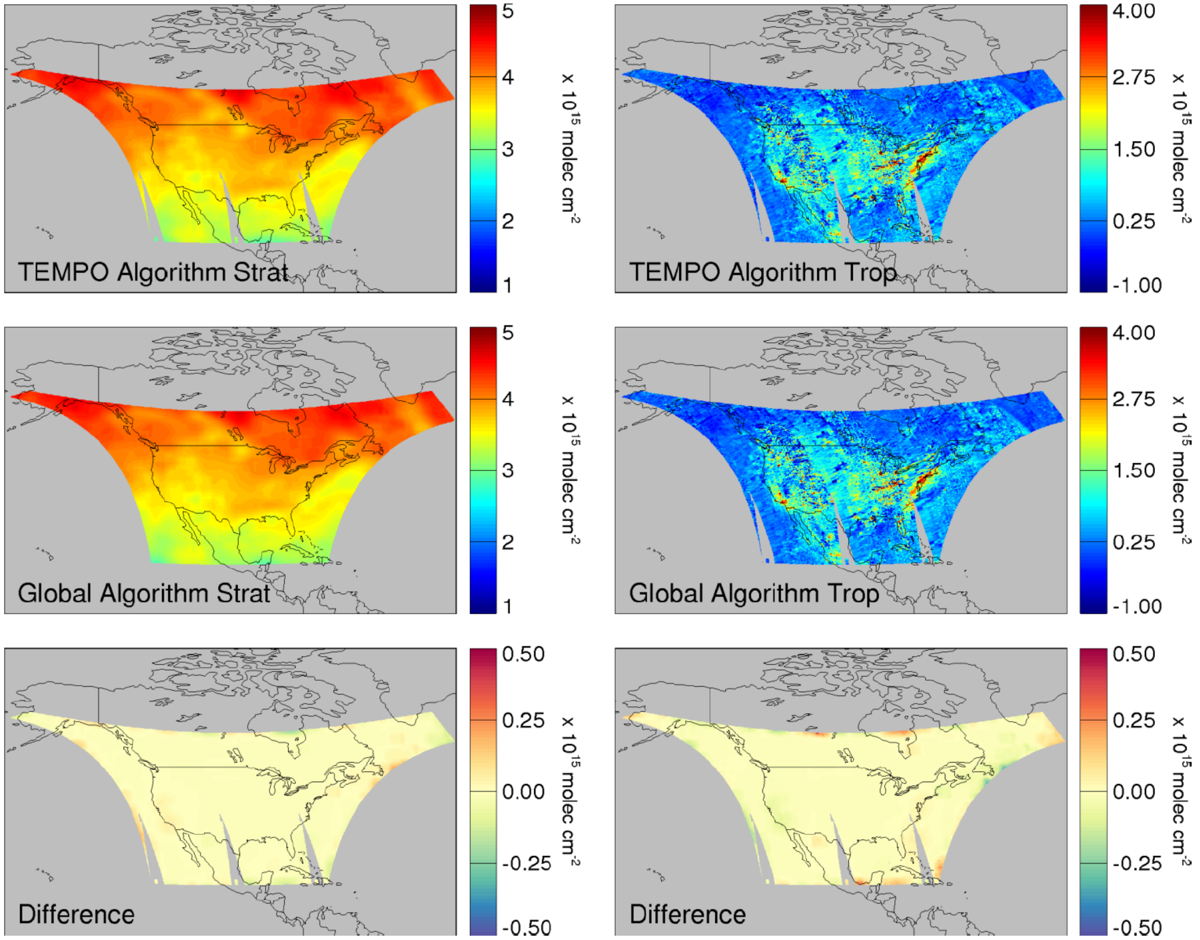
NO$_2$ tropospheric AMF



NO$_2$ total AMF



NO_2 Strat./Trop. Separation



J. Geddes (BU) and R. Martin (Washington Univ.) adapted NASA OMI NO_2 Strat./Trop. Separation algorithm to TEMPO (limited domain)

Example of tropospheric NO_2 synthetic retrievals

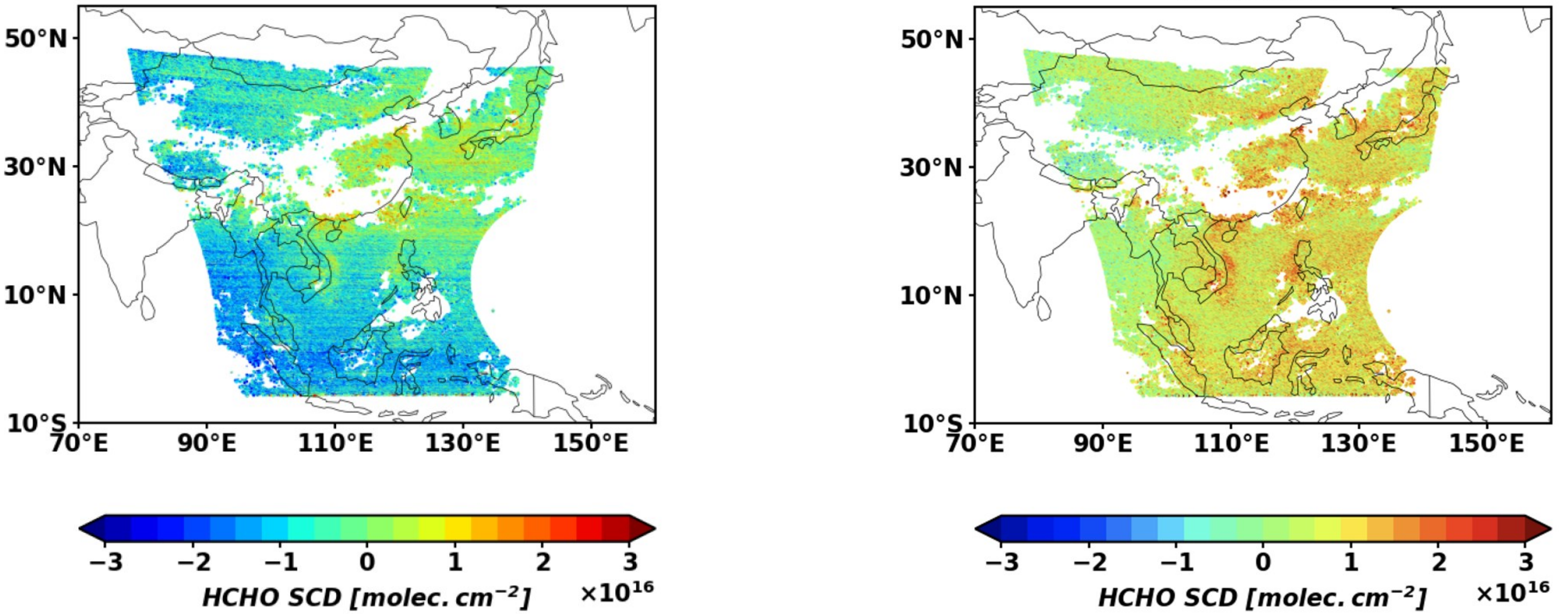
NO_2 tropospheric column

H_2CO corrections

Only upon launch and assessment of TEMPO's performance we would be in a position to decide if H_2CO retrievals could benefit from using radiance reference or other type of corrections. For example, with GEMS a de-striping correction seems to be good enough.

$$SCD_c(i) = SCD(i) - median\big(SCD(i)\big) + median\big(VCD_m(i) \times AMF(i)\big)$$

20210601 0045 UTC



Information included in Level 2 files

Retrieved geophysical quantities plus a priori and ancillary data

NO_2

TEMPO_NO2_L2_V01_20130701T16595...	TEMPO Level 2 nitrogen dioxide product	Local File
geolocation	geolocation	—
latitude	pixel center latitude	Geo2D
latitude_bounds	pixel corner latitude	Geo2D
longitude	pixel center longitude	Geo2D
longitude_bounds	pixel corner longitude	Geo2D
relative_azimuth_angle	relative azimuth angle at pixel center	Geo2D
solar_azimuth_angle	solar azimuth angle at pixel center	Geo2D
solar_zenith_angle	solar zenith angle at pixel center	Geo2D
time	radiance exposure start time	1D
viewing_azimuth_angle	viewing azimuth angle at pixel center	Geo2D
viewing_zenith_angle	viewing zenith angle at pixel center	Geo2D
mirror_step	scan mirror position index	1D
product	product	—
main_data_quality_flag	main data quality flag	Geo2D
vertical_column_stratosphere	stratosphere nitrogen dioxide vertical column	Geo2D
vertical_column_total	nitrogen dioxide vertical column	Geo2D
vertical_column_total_uncertainty	nitrogen dioxide vertical column uncertainty	Geo2D
vertical_column_troposphere	troposphere nitrogen dioxide vertical column	Geo2D
qa_statistics	qa_statistics	—
fit_convergence_flag	radiance fit convergence flag	Geo2D
fit_rms_residual	radiance fit RMS residual	Geo2D
support_data	support_data	—
albedo	surface albedo	Geo2D
amf_cloud_fraction	cloud fraction	Geo2D
amf_cloud_pressure	cloud pressure	Geo2D
amf_diagnostic_flag	nitrogen dioxide air mass factor diagnostic flag	Geo2D
amf_stratosphere	nitrogen dioxide stratospheric air mass factor	Geo2D
amf_total	nitrogen dioxide air mass factor	Geo2D
amf_total_uncertainty	nitrogen dioxide air mass factor uncertainty	Geo2D
amf_troposphere	nitrogen dioxide tropospheric air mass factor	Geo2D
eff_cloud_fraction	effective cloud fraction	Geo2D
fitted_slant_column	nitrogen dioxide fitted slant column	Geo2D
fitted_slant_column_uncertainty	nitrogen dioxide fitted slant column uncertainty	Geo2D
gas_profile	vertical profile of nitrogen dioxide partial column	Geo2D
ground_pixel_quality_flag	ground pixel quality flag	Geo2D
scattering_weights	scattering weights	Geo2D
snow_ice_fraction	Fraction of pixel area covered by snow and/or ice	Geo2D
surface_pressure	surface pressure	Geo2D
terrain_height	terrain height	Geo2D
tropopause_pressure	tropopause pressure	Geo2D
xtrack	pixel index along slit	1D

H_2CO

TEMPO_HCHO_L2_V01_20130701T1723...	TEMPO Level 2 formaldehyde product	Local File
geolocation	geolocation	—
latitude	pixel center latitude	Geo2D
latitude_bounds	pixel corner latitude	Geo2D
longitude	pixel center longitude	Geo2D
longitude_bounds	pixel corner longitude	Geo2D
relative_azimuth_angle	relative azimuth angle at pixel center	Geo2D
solar_azimuth_angle	solar azimuth angle at pixel center	Geo2D
solar_zenith_angle	solar zenith angle at pixel center	Geo2D
time	radiance exposure start time	1D
viewing_azimuth_angle	viewing azimuth angle at pixel center	Geo2D
viewing_zenith_angle	viewing zenith angle at pixel center	Geo2D
mirror_step	scan mirror position index	1D
product	product	—
main_data_quality_flag	main data quality flag	Geo2D
vertical_column	formaldehyde vertical column	Geo2D
vertical_column_uncertainty	formaldehyde vertical column uncertainty	Geo2D
qa_statistics	qa_statistics	—
fit_convergence_flag	radiance fit convergence flag	Geo2D
fit_rms_residual	radiance fit RMS residual	Geo2D
support_data	support_data	—
albedo	surface albedo	Geo2D
amf	formaldehyde air mass factor	Geo2D
amf_cloud_fraction	cloud fraction	Geo2D
amf_cloud_pressure	cloud pressure	Geo2D
amf_diagnostic_flag	formaldehyde air mass factor diagnostic flag	Geo2D
amf_uncertainty	formaldehyde air mass factor uncertainty	Geo2D
background_correction	background correction	1D
destripping_correction	destripping correction	1D
eff_cloud_fraction	effective cloud fraction	Geo2D
fitted_slant_column	formaldehyde fitted slant column	Geo2D
fitted_slant_column_uncertainty	formaldehyde fitted slant column uncertainty	Geo2D
gas_profile	vertical profile of formaldehyde partial column	Geo2D
ground_pixel_quality_flag	ground pixel quality flag	Geo2D
reference_sector_correction	reference sector correction	Geo2D
scattering_weights	scattering weights	Geo2D
snow_ice_fraction	Fraction of pixel area covered by snow and/or ice	Geo2D
surface_pressure	surface pressure	Geo2D
terrain_height	terrain height	Geo2D
xtrack	pixel index along slit	1D

THANKS FOR YOUR ATTENTION

TEMPO Level 3 algorithms are ready to produce data up a year from now!!!

If you have questions please contact one of us:
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Xiong Liu (xliu@cfa.harvard.edu)
Caroline Nowlan (cnowlan@cfa.harvard.edu)
Gonzalo González Abad (ggonzalezabad@cfa.harvard.edu)

Back up slides

TEMPO Data Products

Level	Product	Algorithm	Major Outputs	Res km[2] **	Freq/Size
L0	**Digital counts**	Raw to L0	Reconstructed/reformatted digital counts	2.0 x 4.75	Daily/hourly
L1-b	**irradiance**	SAO L0-1	Calibrated & quality flags		daily
	radiance	SAO L0-1	Geolocated,calibrated, viewing,geolocation&quality flags	2.0 x 4.75	Hourly, granule
L2	**Cloud**	OMCLDRR*	Cloud fraction, cloud pressure	2.0 x 4.75	Hourly, granule
	O_3 profile	SAO O3 profile	O3 profile, total/strat/trop/0-2 km O3 column, errors, a priori, AKs	8.0 x 4.75	Hourly, granule
	Total O_3	TOMS V8.5	Total O3, AI, cloud fraction	2.0 x 4.75	Hourly, granule
	NO_2	SAO trace gas, BU strat/trop sep.	SCD, strat./trop. VCD, error, shape factor, scattering weights	2.0 x 4.75	Hourly, granule
	H_2CO	SAO trace gas	SCD, VCD, error, shape factor, scattering weights	2.0 x 4.75	Hourly, granule
	$C_2H_2O_2$	SAO trace gas		2.0 x 4.75	Hourly, granule
	H_2O	SAO trace gas		2.0 x 4.75	Hourly, granule
	BrO	SAO trace gas		2.0 x 4.75	Hourly, granule
	SO_2	OMSO2 PCA	SCD, VCD (PBL,TRL,TRM,TRU,STL)	2.0 x 4.75	Hourly, granule
	Aerosol	OMAERUV	AAI, AOD, SSA	8.0 x 4.75	Hourly, granule
L3	**Gridded L2**	SAO L2-3	Same as L2	TBD	Hourly, scan
L4	**UVB**	OM UVB	UV irradiance, erythemal irradiance, UVI	TBD	Hourly, scan

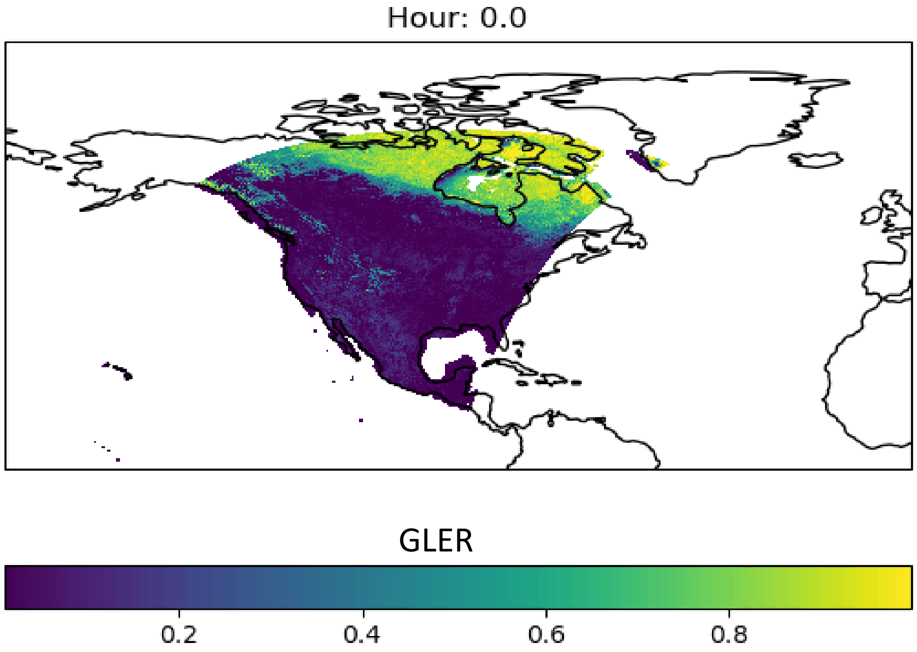
*Algorithm may be changed to use NASA GSFC's O_2-O_2 cloud algorithm. ** Spatial resolution at center of FOR.
This table lists products that are likely ready for operational processing and can be archived.

TEMPO Algorithm Teams

Operational Algorithm	Personnel
Raw to L0	John Davis
L0-1b	Xiong Liu, John Houck, Dave Flittner, Nischal Mishra, Chris Chan Miller
Ozone profile	Xiong Liu, Juseon Bak
Total ozone	Joanna Joiner, Dave Haffner
Nitrogen dioxide	Caroline Nowlan, Gonzalo González Abad, Jeff Geddes, Chris Chan Miller
Formaldehyde	Gonzalo González Abad, Caroline Nowlan, Chris Chan Miller
Glyoxal	Chris Chan Miller, Gonzalo González Abad
Sulfur dioxide	Can Li, Nicolay Krotkov
Clouds	Joanna Joiner, Alexander Vasilkov
Aerosols	Omar Torres

Operational implementation and IT support @ SAO Science Data Processing Center (SDPC) by John Houck and Ewan O'Sullivan

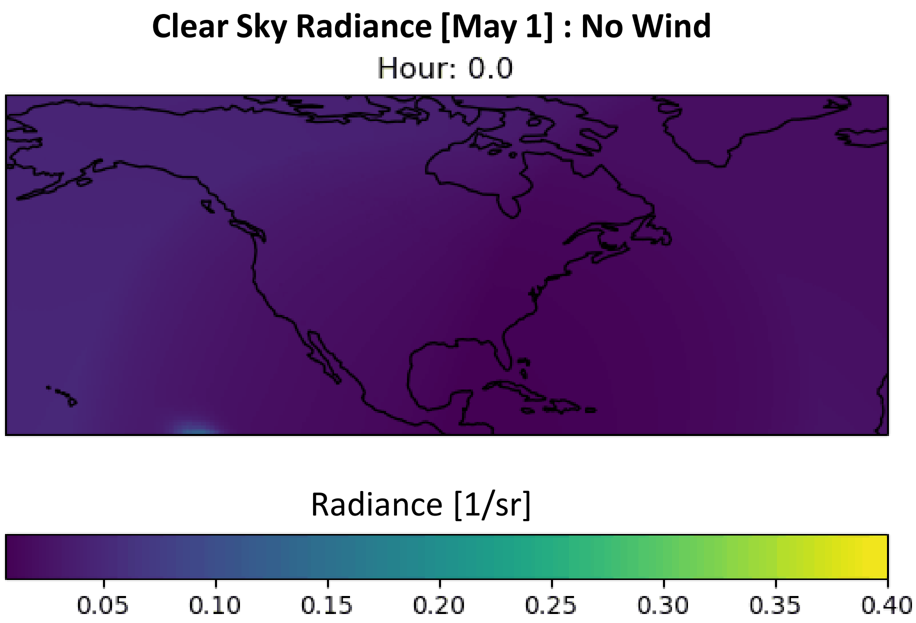
GLER OVER LAND USES A 20-YEAR MODIS CLIMATOLOGY SEGREGATING BY SNOW COVERED AND SNOW FREE CASES



Information from the Iterative Multisensor Snow and Ice Mapping System (IMS) is used to identify snow/ice pixels.

Hyperspectral extension of MODIS bands is achieved by inverting GLER at 4 MODIS bands, using a probabilistic model trained on SCHIAMACHY/USGS reflectance spectra.

GLER OVER OCEANS USES VLIDORT NEWCM GLINT KERNEL (FUNCTION OF WIND/CHLOROPHYLL)



To precompute tables we used MODIS chlorophyll climatology.

The ocean GLER tables include wind dependence; operationally the algorithm uses winds from GEOS-FP.

We are still looking for the best approach to account for sea ice.