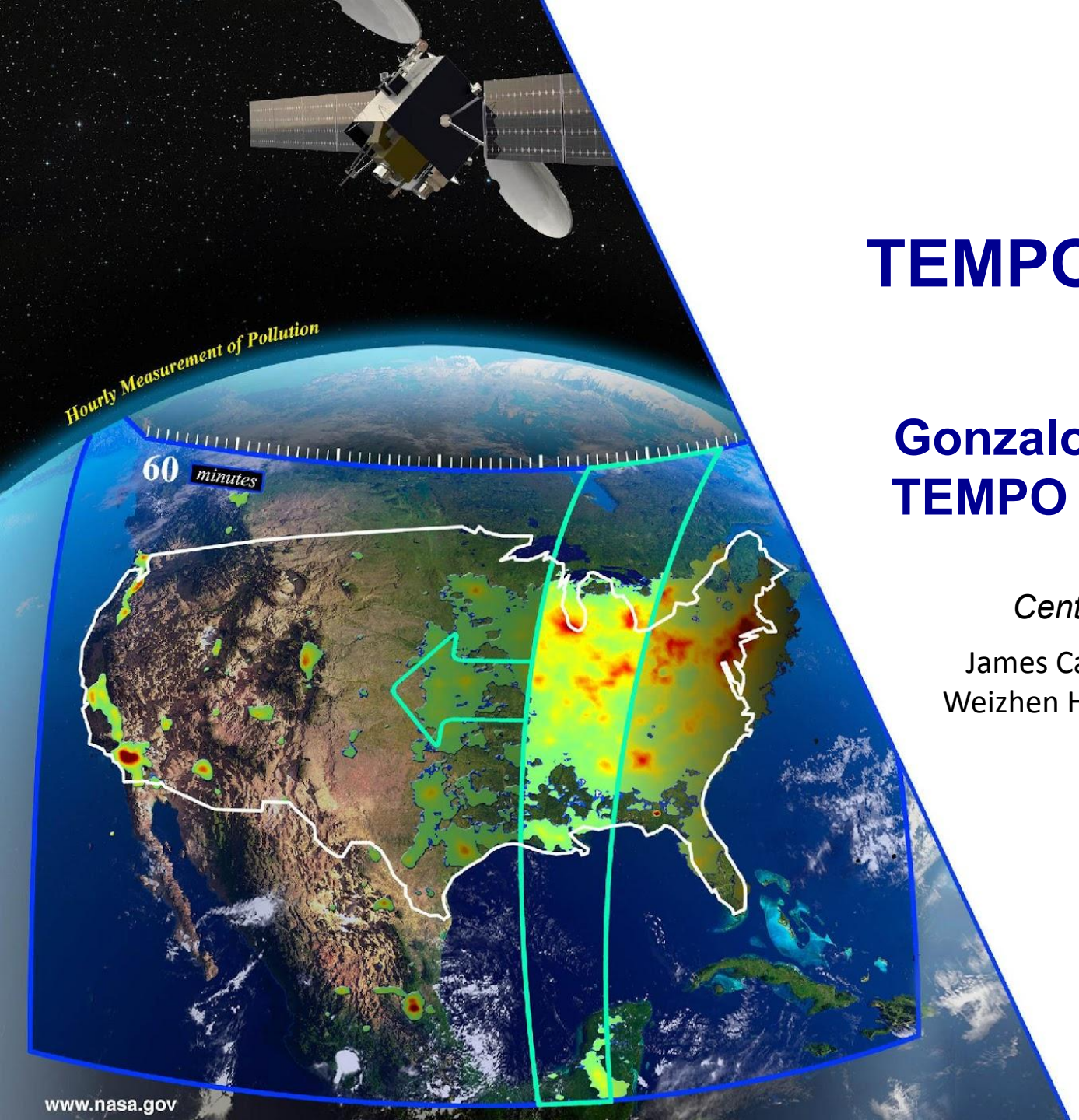


Tropospheric Emissions:
Monitoring of Pollution

TEMPO NO_2 and HCHO retrieval status update

Gonzalo González Abad on behalf of the TEMPO Science Data Processing Center Team

Center for Astrophysics | Harvard & Smithsonian

James Carr, Kelly Chance, Heesung Chong, Jean Fitzmaurice, Weizhen Hou, John Houck, Xiong Liu, Caroline Nowlan, Junsung Park, Raid Suleiman, Huiqun Wang

GeoXO ACX Meeting

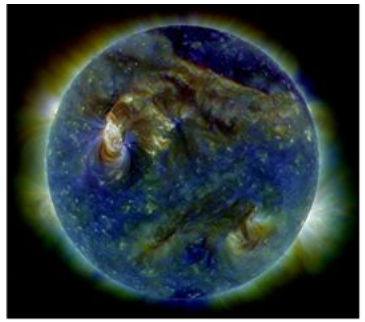
May 7, 2024

Smithsonian

TEMPO NO_2 and HCHO retrieval basics

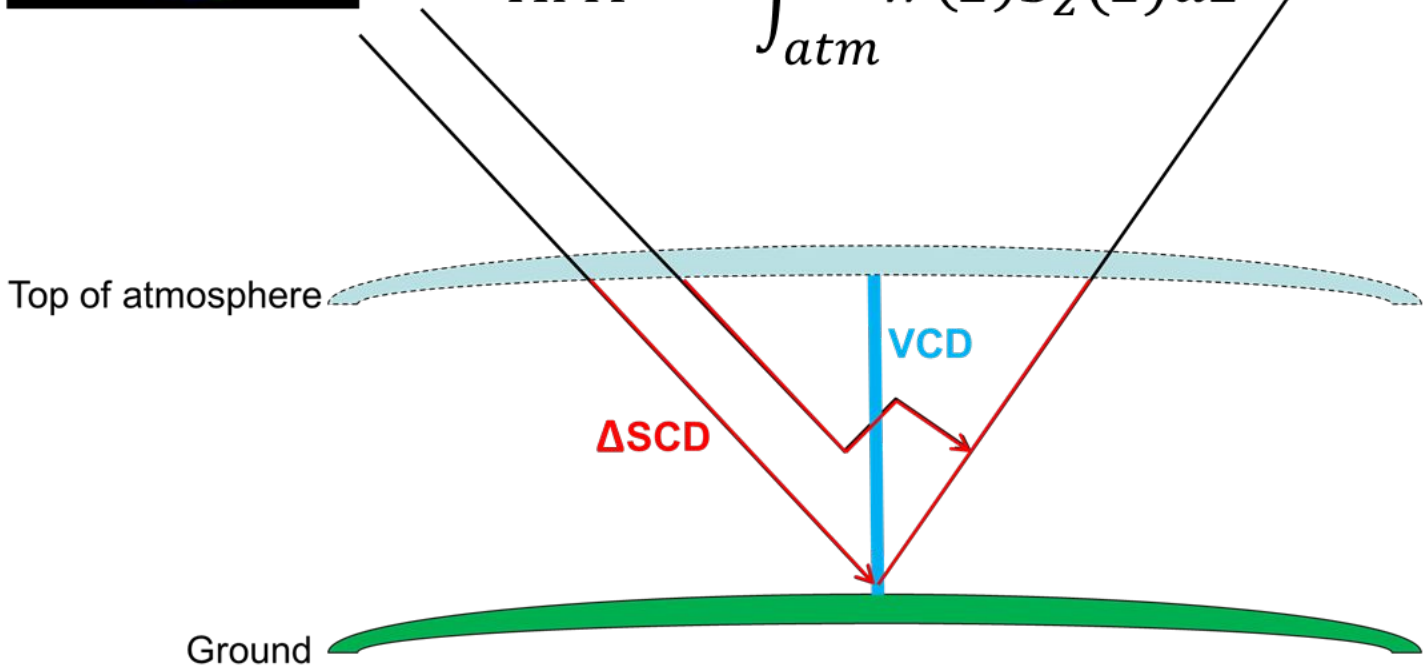
TEMPO NO_2 and HCHO share the differential slant column fit (also used for cloud O_2-O_2 columns), and air mass factor calculation.

Then NO2 columns undergo stratospheric/tropospheric separation and HCHO columns are corrected to account for the use of radiance reference source spectra.



$$VCD = \frac{\Delta SCD + SCD_R}{AMF}$$

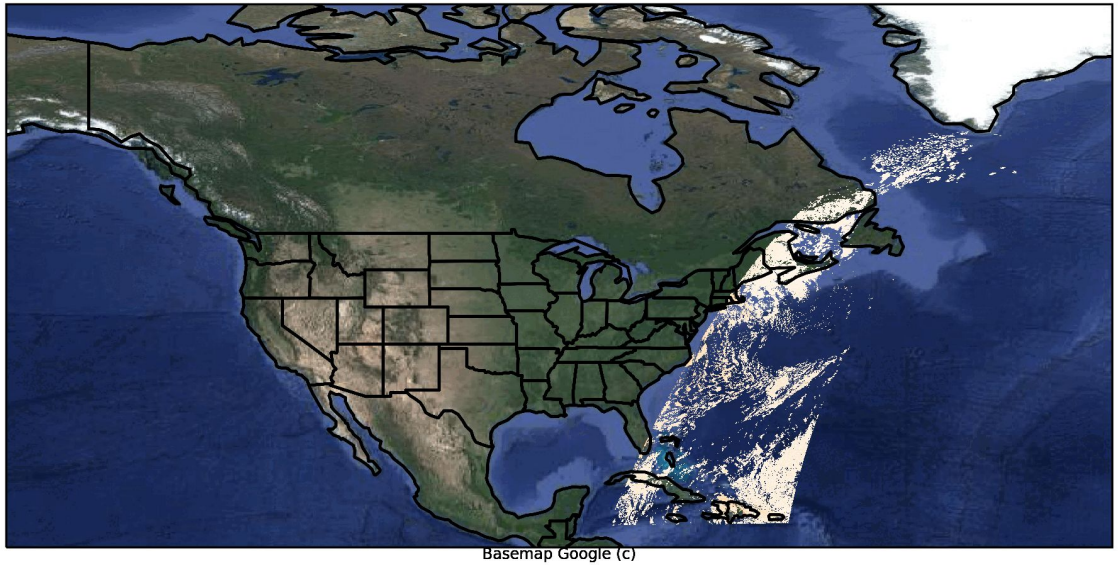
$$AMF = \int_{atm} w(z) S_z(z) dz$$



A couple of examples but much more in the validation talks

TEMPO tropospheric NO_2 (v2)
2 November 2023

Scan 001 (11:41:46 UTC)



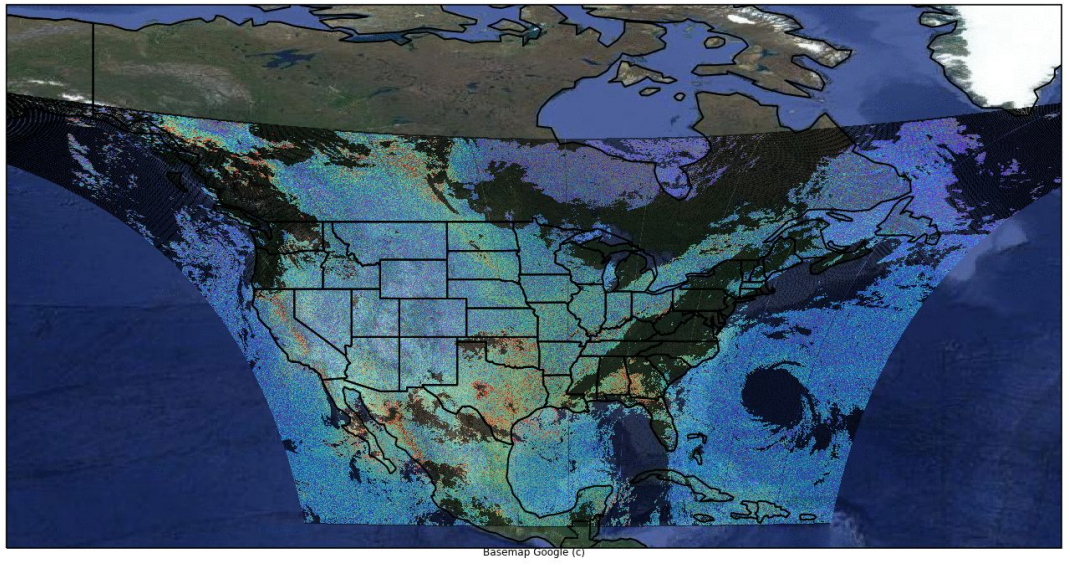
molecules/cm^2

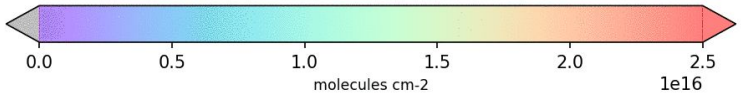
[credit: Caroline Nowlan]

TEMPO HCHO (v1)
29-31 August 2023

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

vertical_column

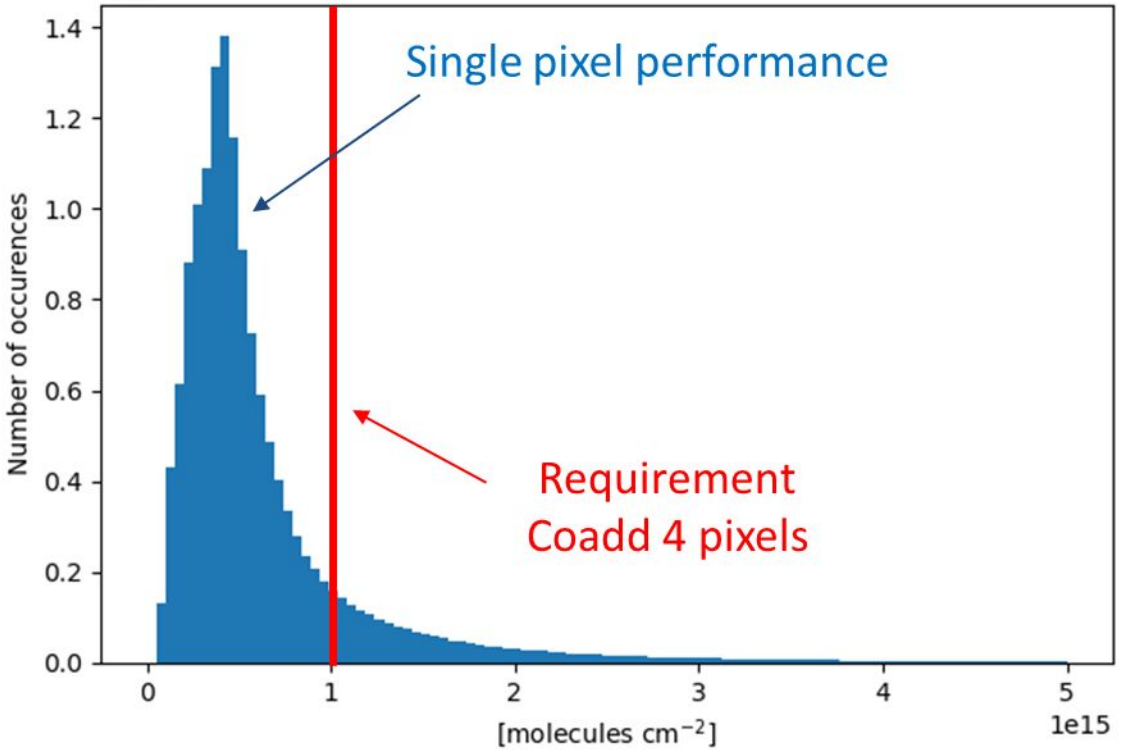




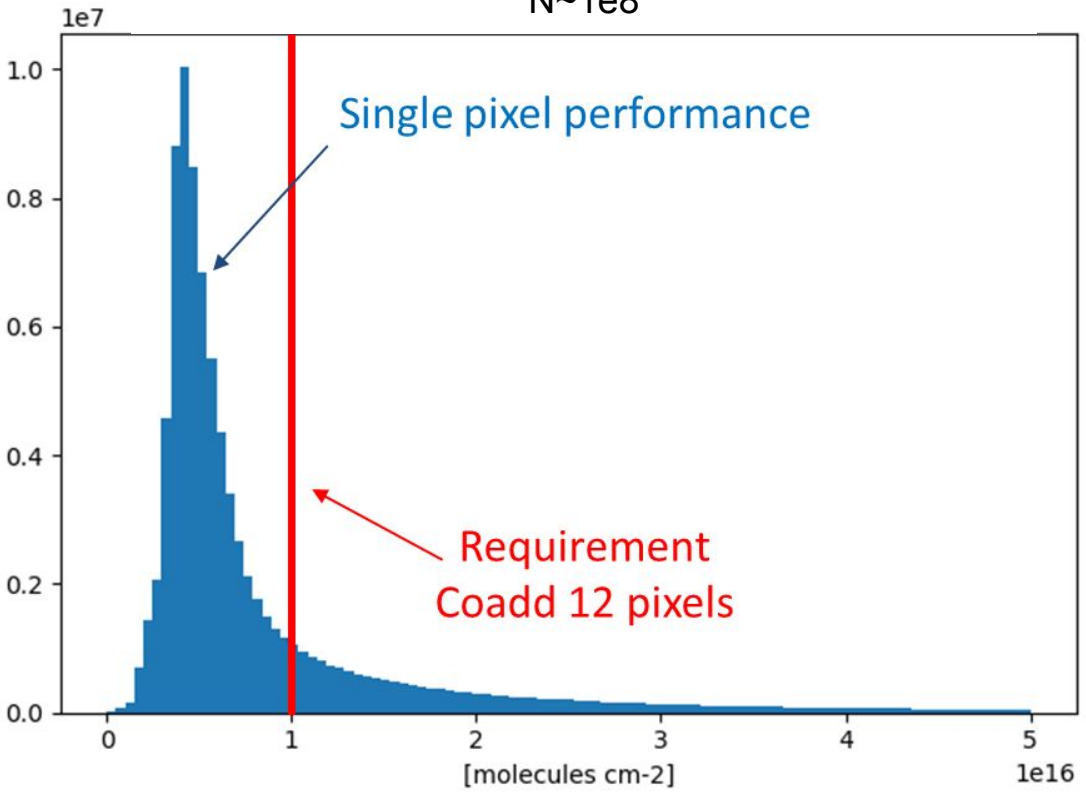
Unofficial Data: Not for Public Release

Both, NO2 and HCHO fulfill the fitting uncertainty requirements

NO2 tropospheric vertical column uncertainty (fitting)
N~1e7



HCHO vertical column uncertainty (fitting)
N~1e8



TEMPO NO_2 meets the requirement for 95% of cloud-free scenes with **no pixel coadding**!
TEMPO HCHO meets the requirement for 93% of cloud-free scenes with **no pixel coadding**!

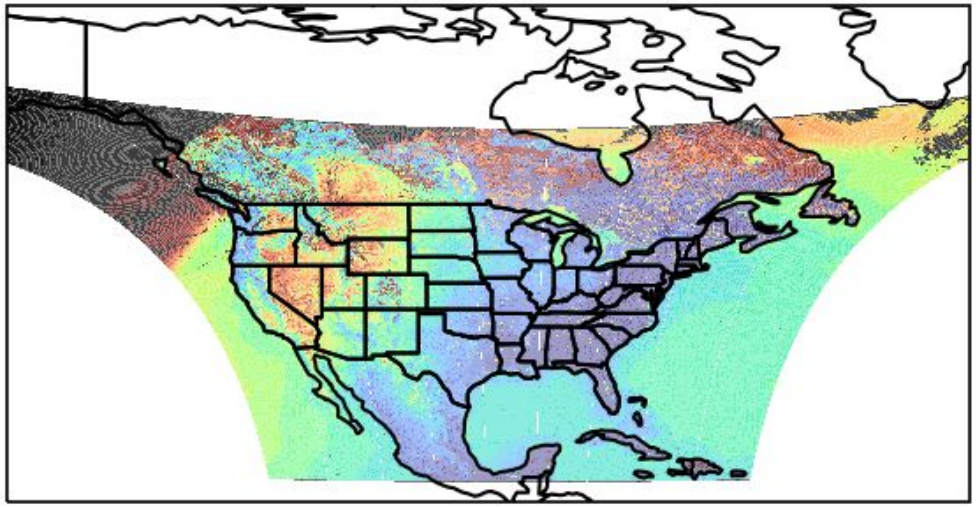
Algorithm updates since version 1

- **SDPC v4.3 (V2)**
  - Include temperature correction in NO_2 AMF calculation
  - Tropopause layer determination bug fix
  - Carry on retrieval for a given North-South position even if radiance wavelength calibration fails
  - Increase spatial resolution of Level 3 files to 0.02° x 0.02°
  - Address some Level 2 & 3 file format feedback from ASDC
- **SDPC v4.4 (V3) & Level 2-3 release: ~May 20, 2024**
  - New GLER LUTs (v6.0->v6.1, snow free + 100% snow, quality flag 2 & 5, fill in gaps via interpolation)
  - Revisit logic to calculate surface albedo in the presence of ice and snow
  - Extrapolate scattering weights for the bottom layers if necessary
  - Avoid including residual stratospheric air masses in tropospheric AMF calculation
  - Use TSIS solar spectrum in wavelength and slit calibrations
  - Perform retrievals up to SZA 90
  - Update main data quality flag (AMF > 6 as suspect, ~SZA 70 + VZA 70)
  - Revisit convergence flag & AMF diagnostic flag
  - Add temperature profile to output (for AMF)
  - Move total NO$_2$ vertical column to support_data group

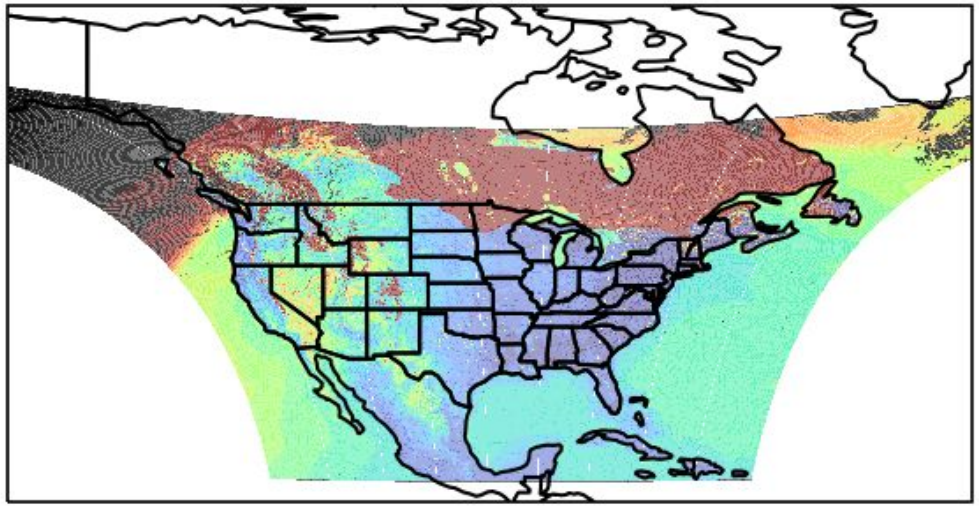
Current issues keeping us awake
Surface Reflectance Climatology

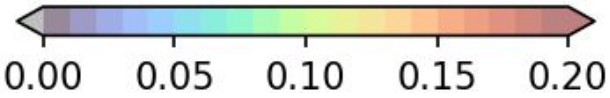
November 11, 2023: scan 006

Version 2 albedo



Version 3 albedo





Over snow version 3 performance is much better

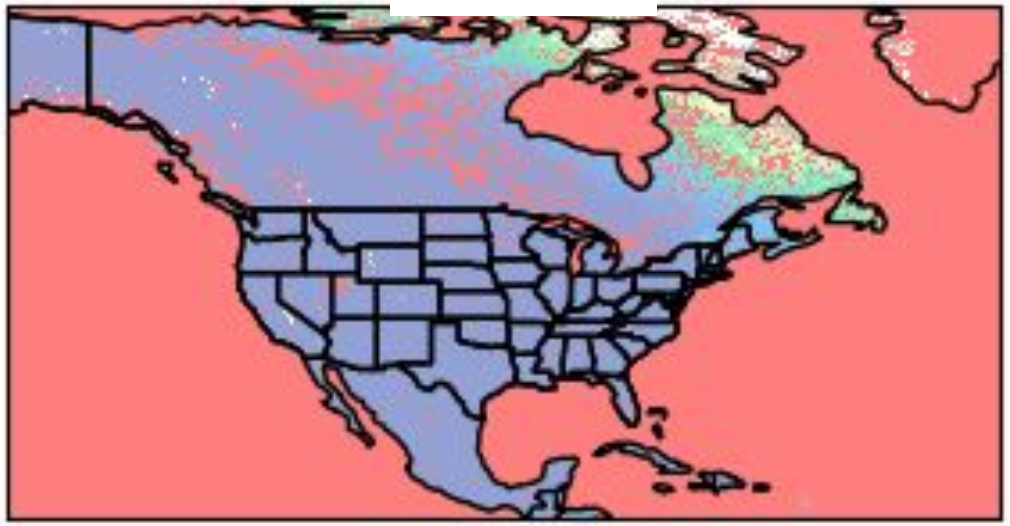
In the Western part of the FOR, in the absence of snow version 3 is much lower and this change is associated to the MODIS BRDF version (6.0 vs 6.1)

Current issues keeping us awake
Surface Reflectance Climatology

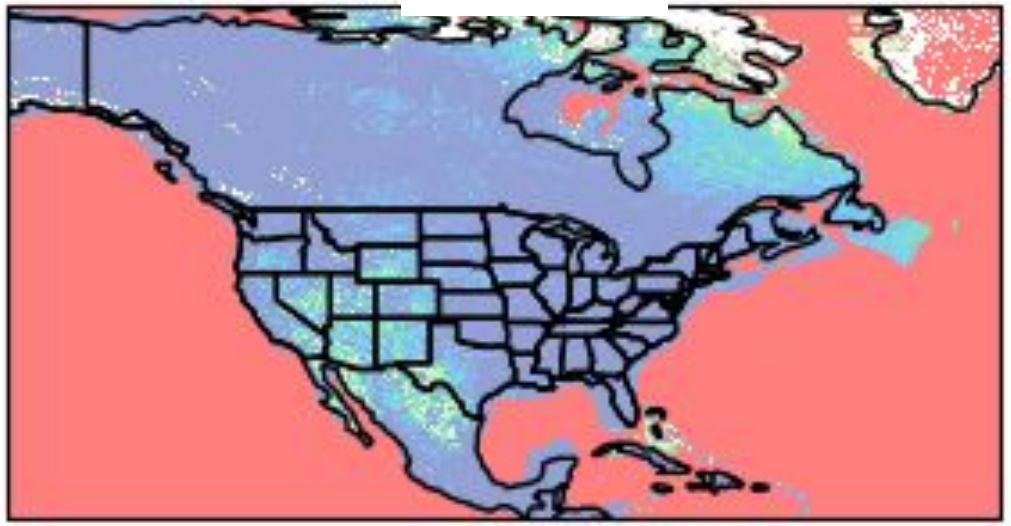
Land GLER LUT at 466nm, DOY 167

0.0h

Version 2



Version 3



The differences are remarkable, at some times of the day

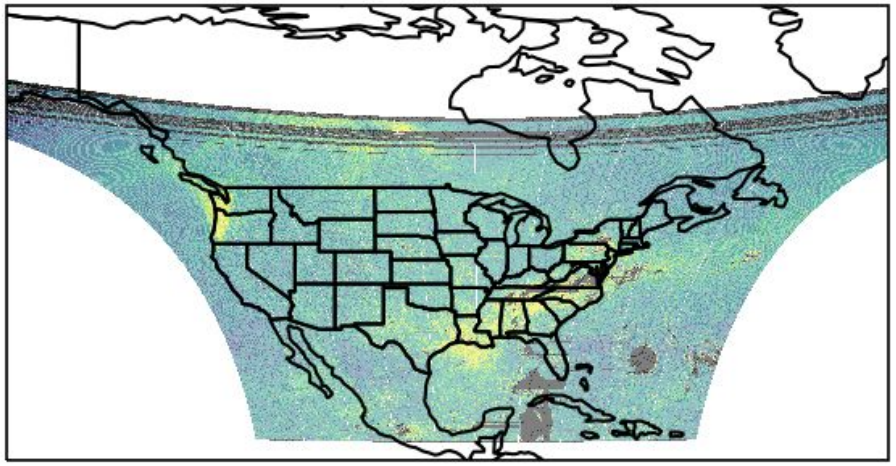
As more observations become available, we need to derive a TEMPO GLER product!!!

Unofficial Data: Not for Public Release

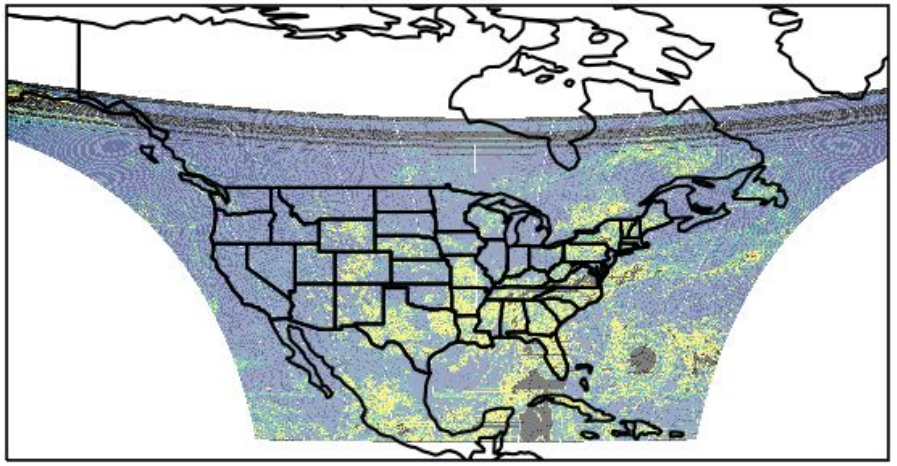
Current issues keeping us awake
Uncertainty in Inhomogeneous Scenes

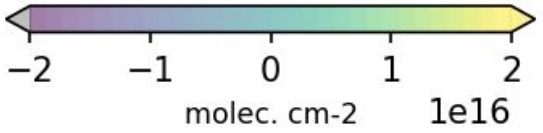
August 28, 2023: scan 009

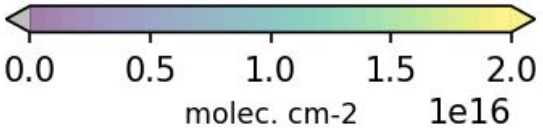
HCHO SCD



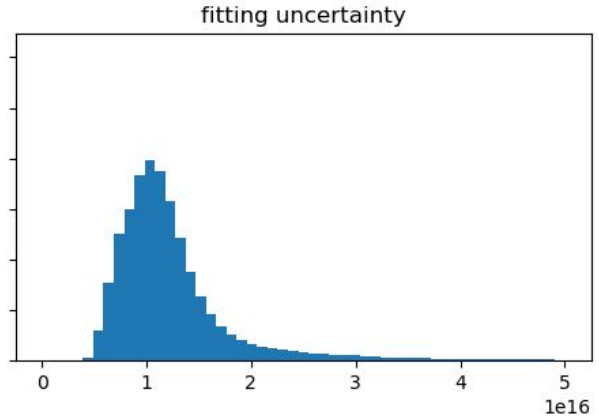
HCHO UNC

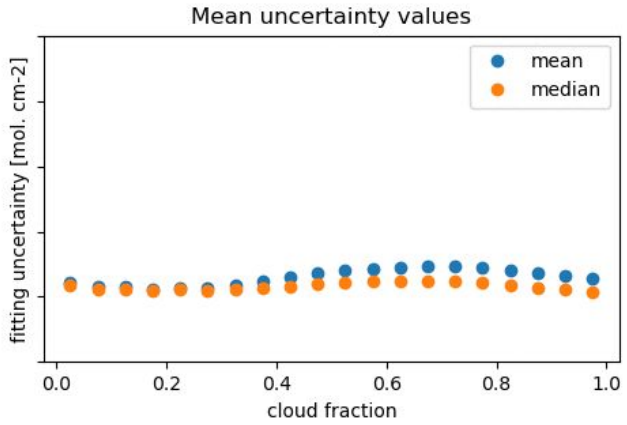






August 28-30 scans





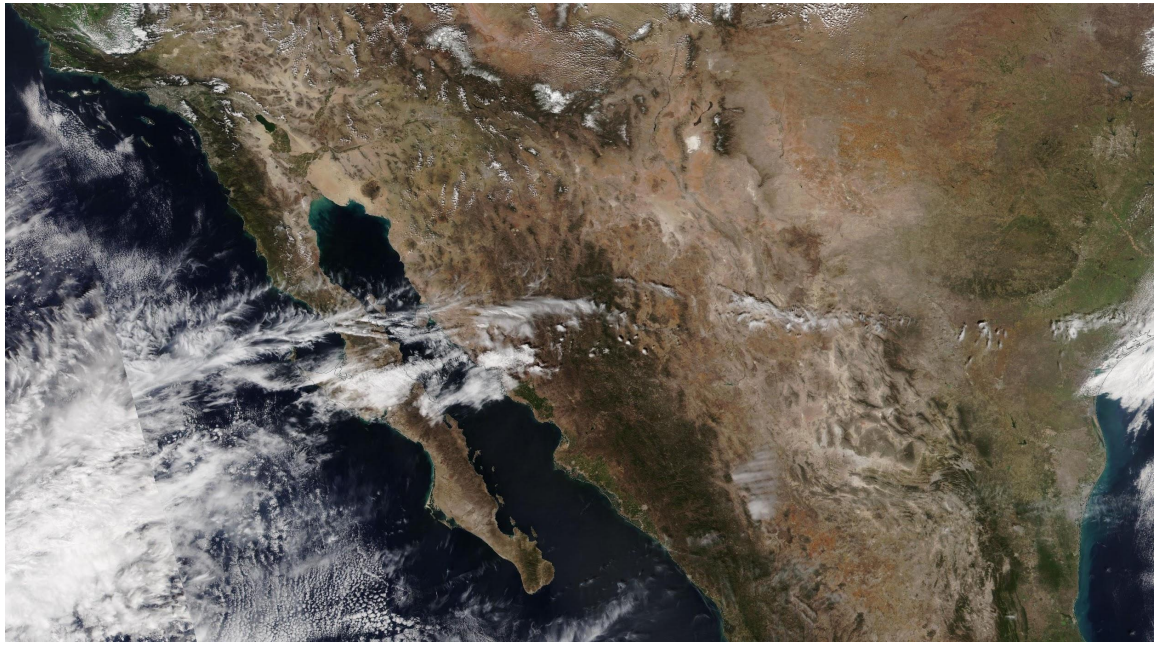
We believe that inhomogeneous illumination of the instrument slit results in enhanced fitting uncertainties and biases in the retrieved slant columns. To mitigate this problem, we will investigate using pseudo-absorbers derived from fitting residuals or derivatives of the slit function.

For now, we aware of the issue and treat pixels with cloud radiance fraction bigger than ~0.2 (for HCHO) and ~0.15 (for NO_2) with caution.

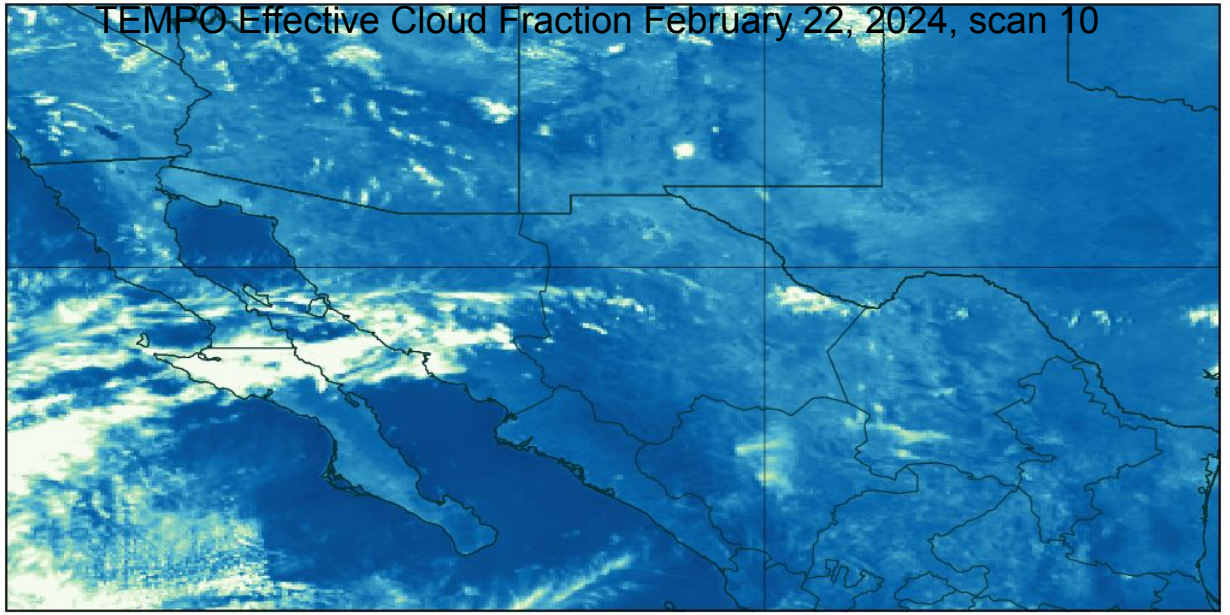
Unofficial Data: Not for Public Release

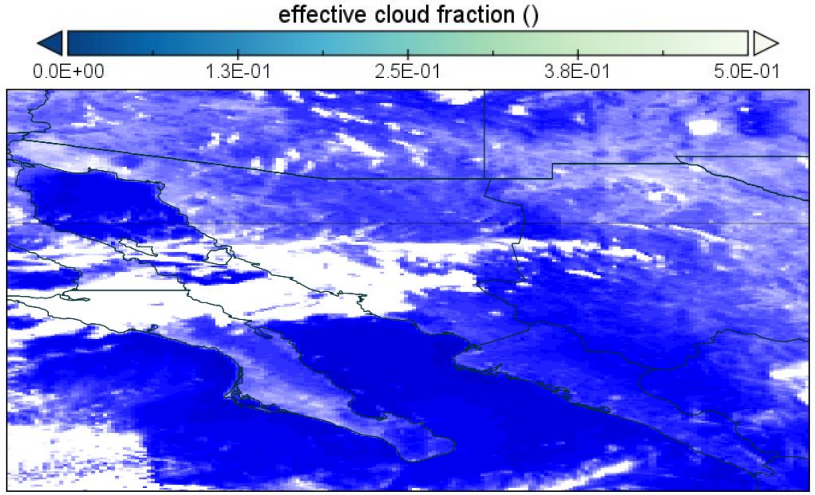
Current issues keeping us awake
Cloud Fraction Histogram

WorldView VIIRS February 22, 2024



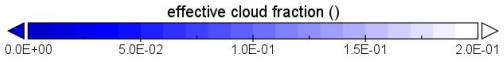
TEMPO Effective Cloud Fraction February 22, 2024, scan 10



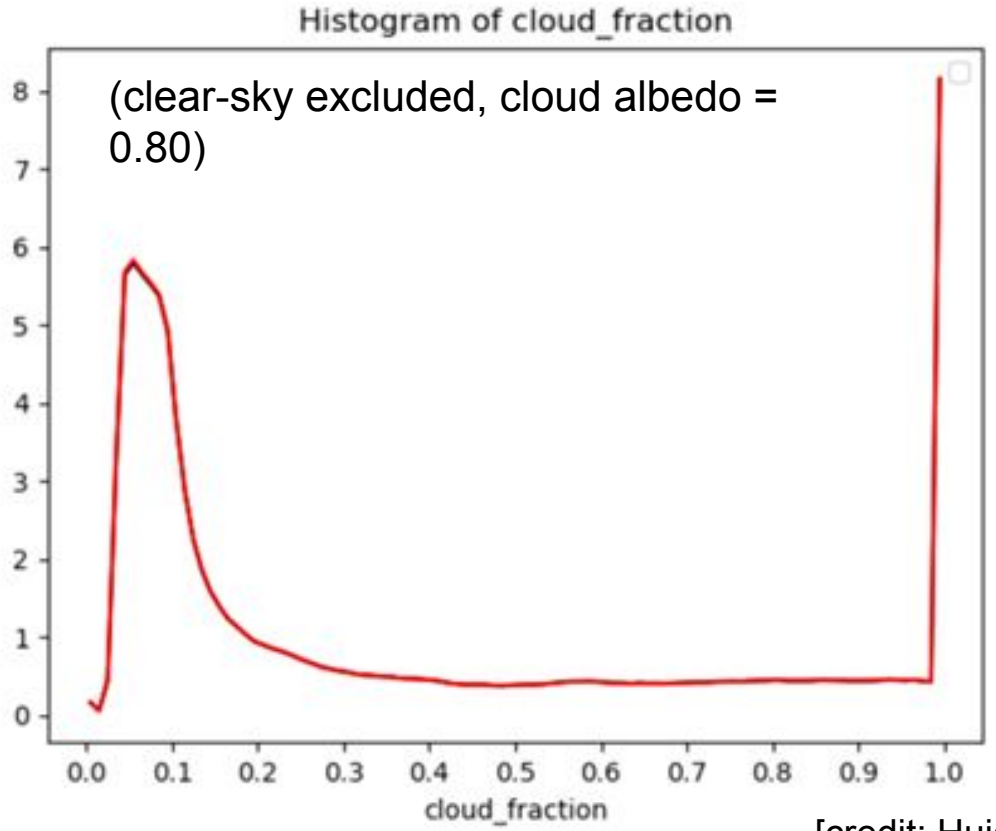


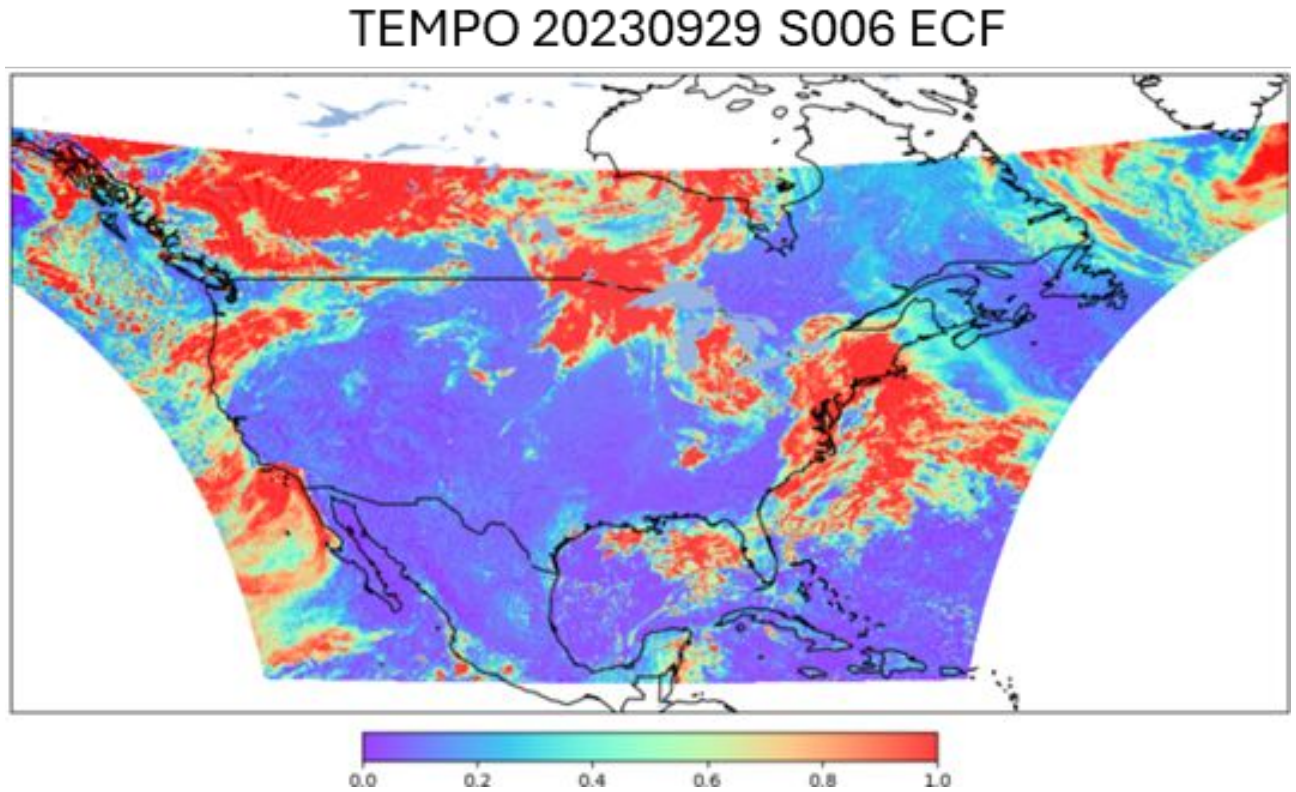
Clear-sky cloud fraction
Topographic signatures
Land-water transition

Unofficial Data: Not for Public Release



Current issues keeping us awake
Cloud Fraction Histogram





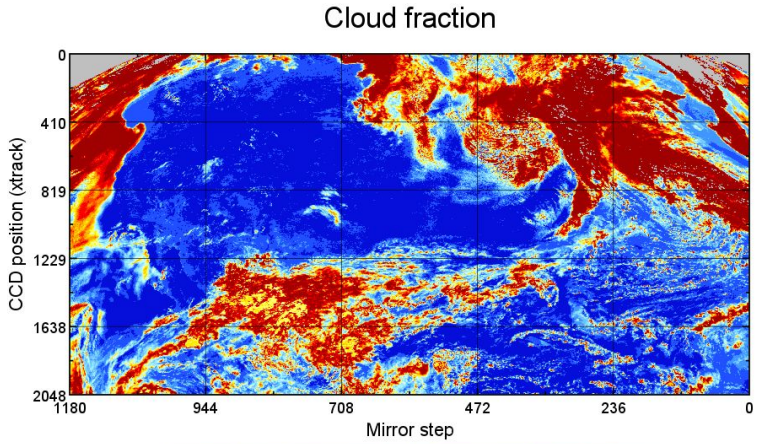
[credit: Huiqun Wang]

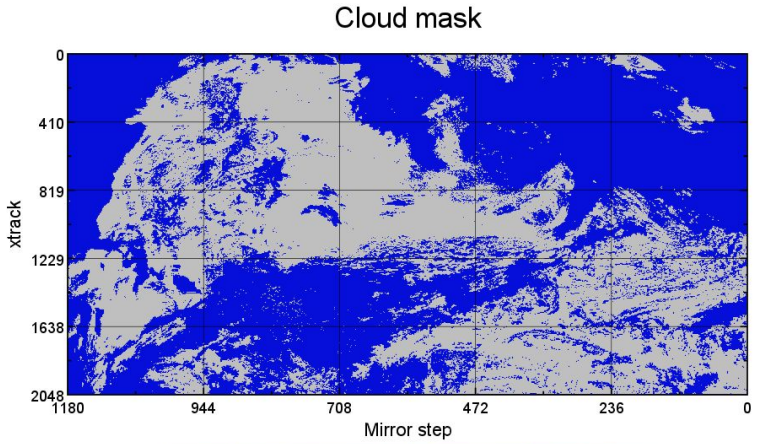
Histogram of cloud fractions shows a local peak between 0.05 and 0.1 situation that could be linked with possible biases in the normalized radiances and the a priori GLER. We are actively investigating both.

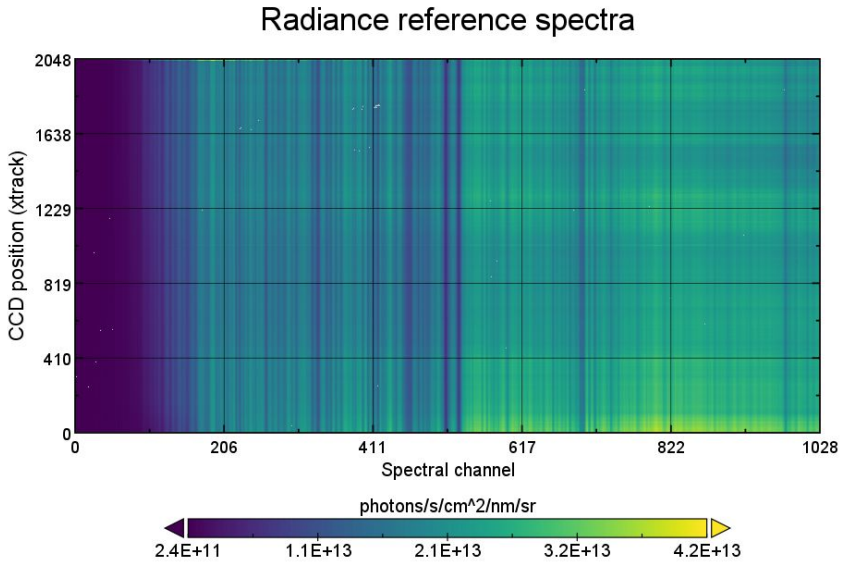
Unofficial Data: Not for Public Release

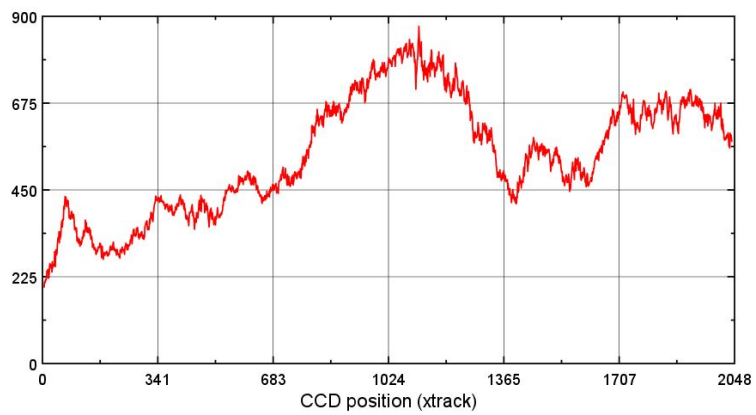
Current issues keeping us awake
HCHO Radiance Reference

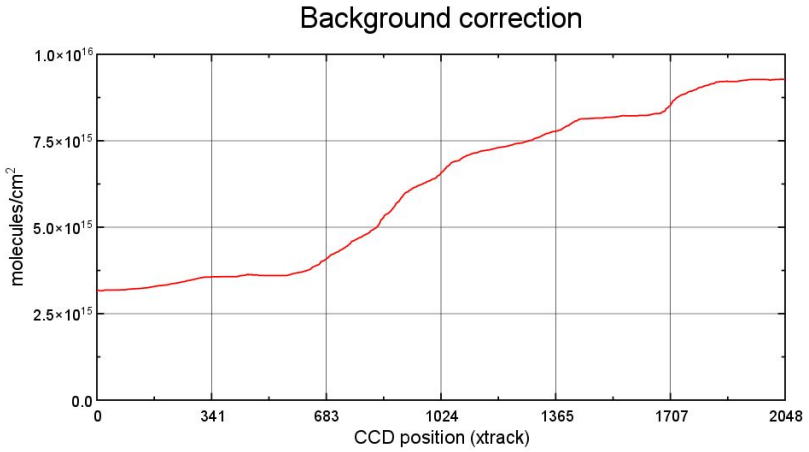
It is better to use pixels with small cloud fractions (< 50%) in the radiance reference calculations (similar to GEMS). Currently calculation is done on a scan basis, but it results in missing data for some xtrack positions







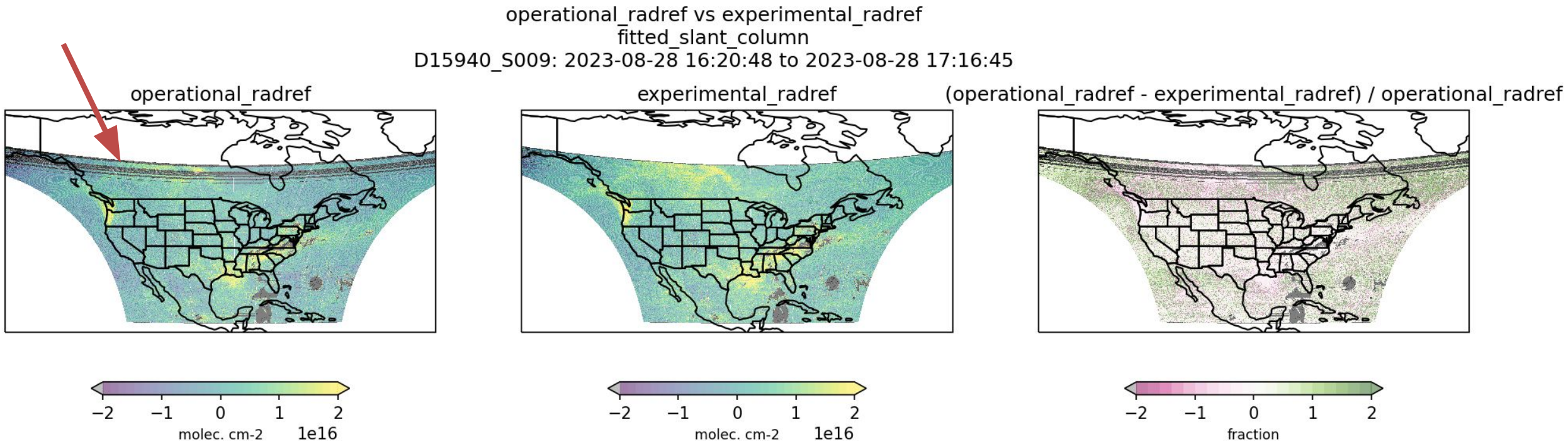




Unofficial Data: Not for Public Release

Current issues keeping us awake
Radiance Reference

So, we are developing a more complex approach taking into consideration GEOS-CF modeled HCHO and multiple days of observations.



Unofficial Data: Not for Public Release

Next in the pipeline

- Improve GLER tables
- Finalize radiance reference experiments and implement operationally
- Add clear sky AMF and scattering weights to level 2 (and maybe level 3) files
- Improve fittings in inhomogeneous scenes
- Mitigation of cloud fraction bias which could benefit from improvements in radiometric calibration, GLER and if necessary, reference tables

Thanks for your attention

Questions?

Air mass factor calculation inputs

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 (0.05° resolution) using OMI GSFC team methodology over land (Fasnacht et al., 2019) and water (Qin et al., 2019). Derived from MODIS BRDF v6.1, extended to shorter wavelengths 340 nm (HCHO) using visible surface reflectance EOFs updated from Zoogman et al. (2016) and SCIAMACHY reflectance climatologies.
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)

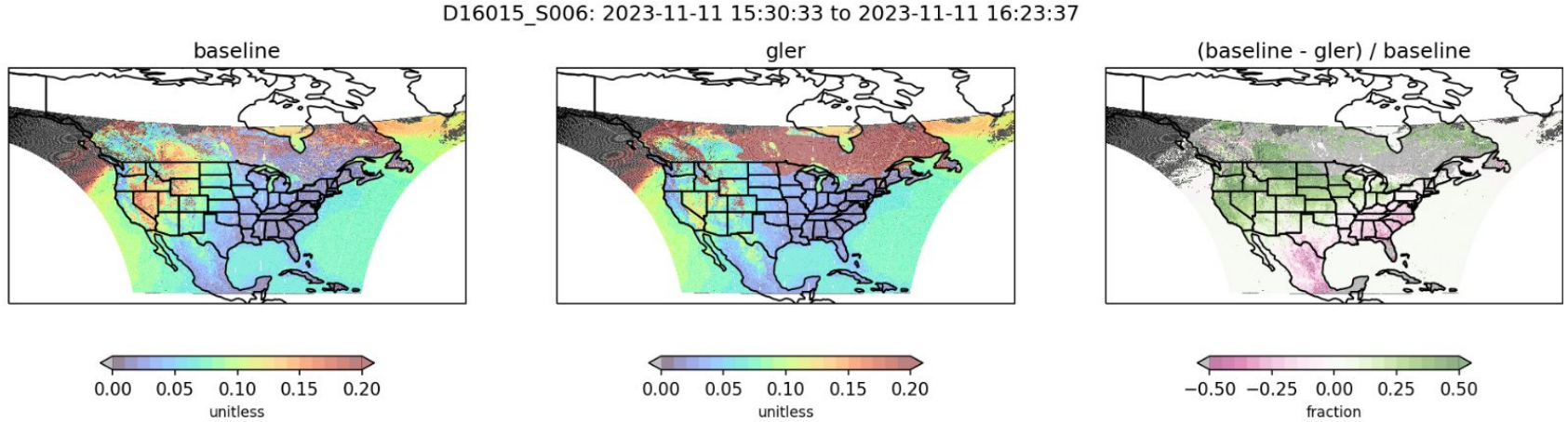
Differential slant column spectral fit set up

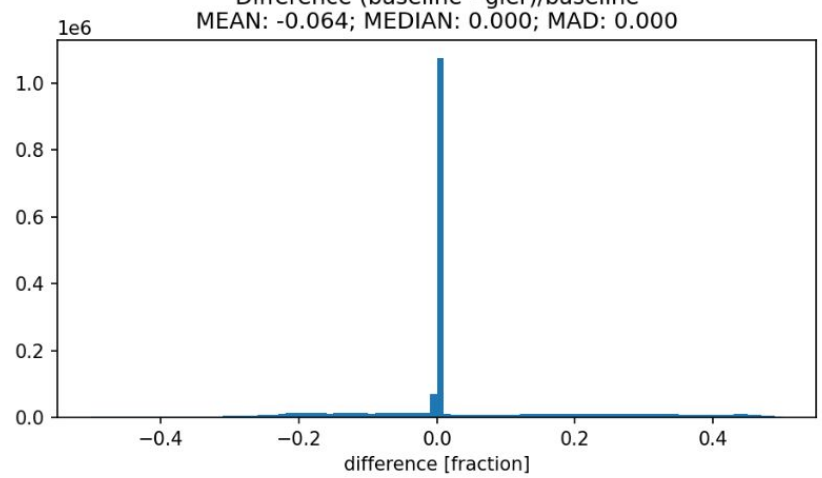
Fitting window	328.5 - 356.5 nm
I_0	CCD position dependent radiance reference calculated using same scan
Baseline polynomial	3rd order
Scaling polynomial	3rd order
Solar reference spectrum	Chance and Kurucz (2010)
Raman Scattering	Derived using Chance and Spurr (1997)
Undersampling correction	Derived using Chance et al. (2005)
O_3	Serdyuchenko et al. (2014) at 223K and 243K
NO_2	Vandaele et al. (1998) 220K
O_2-O_2	Finkenzeller and Volkamer (2022) 293K
BrO	Wilmouth et al. (1999) 228K
HCHO	Chance and Orphal (2011) 300K

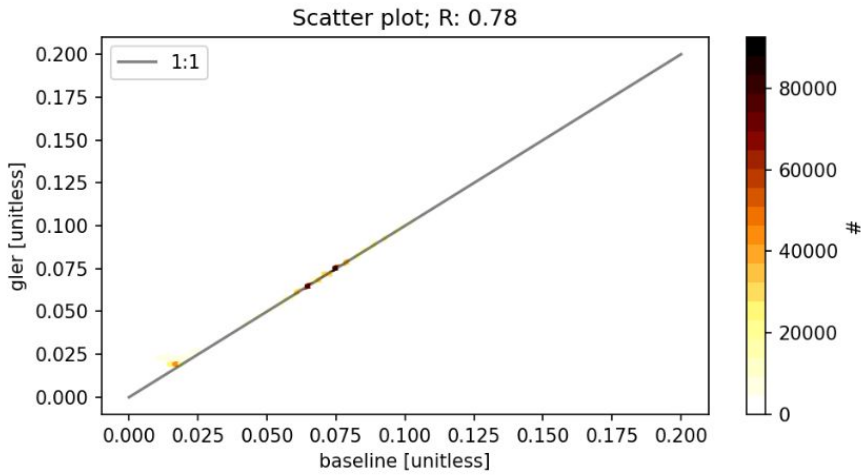
$$I = \left[(aI_o + \sum_i \alpha_i X_i)e^{-\Sigma_j \alpha_j X_j} + \sum_k \alpha_k X_k\right] ScalPoly + BasePoly$$

V3 changes in nitrogen dioxide and formaldehyde cloud parameters

Version 3 (release planned May 20): Updated GLER tables affect AMF calculations and retrieved cloud fraction (particularly important over snow-ice areas)



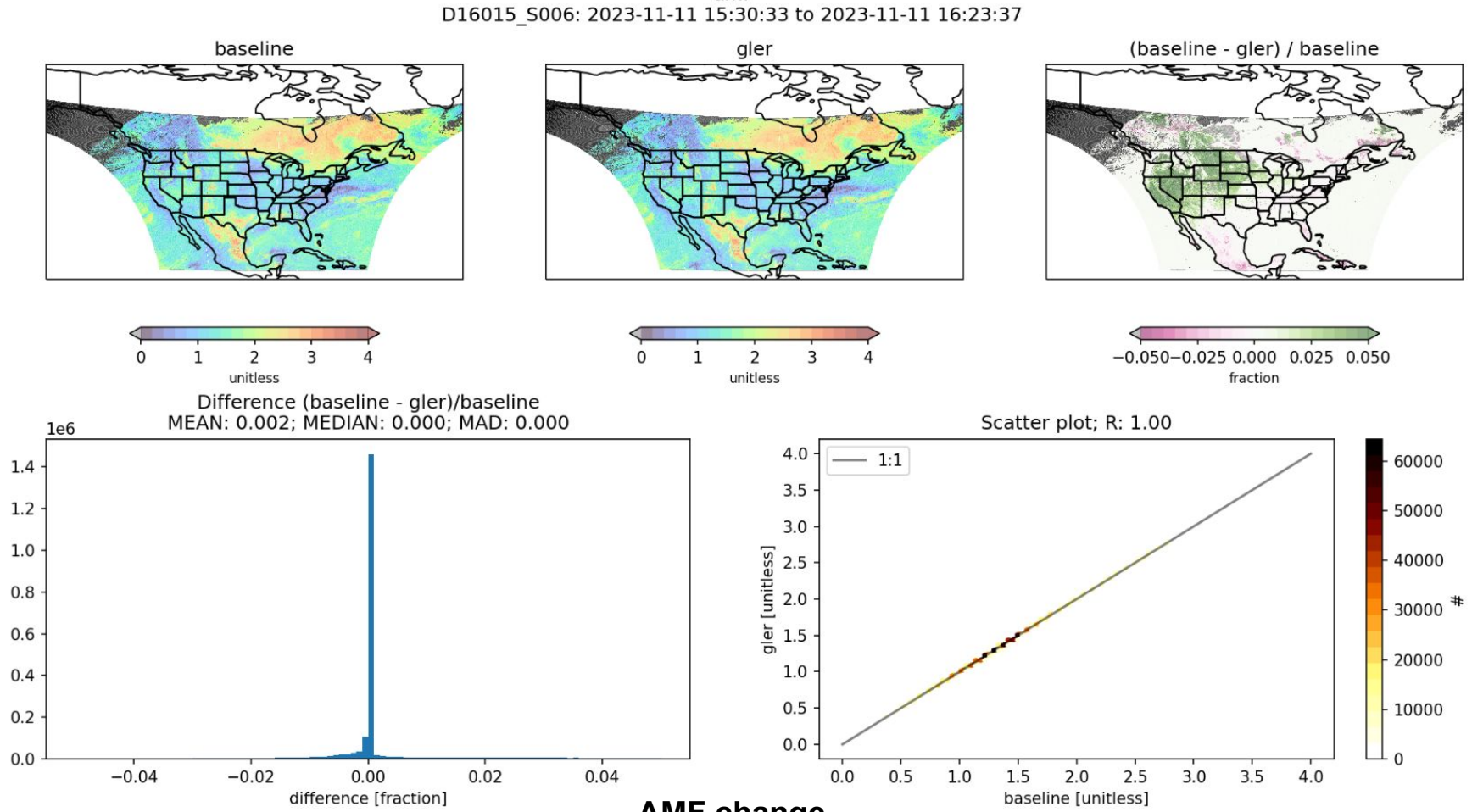




- GLER changes over snow/ice regions are significant. Before we had too many gaps in the GLER tables.
- Changes elsewhere associated with MODIS BRDF version and temporal interpolation.
- Direction of change depends on time of day and year.
- Affects AMF calculations and cloud fraction retrievals

V3 changes in nitrogen dioxide and formaldehyde cloud parameters

Version 3 (release planned May 20): Updated GLER tables affect AMF calculations and retrieved cloud fraction (particularly important over snow-ice areas)



AMF change