SAO Tropospheric Ozone Retrieval Algorithms for OMI and TEMPO

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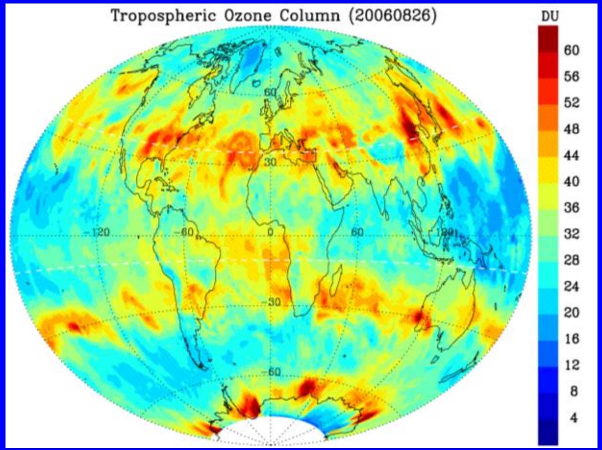
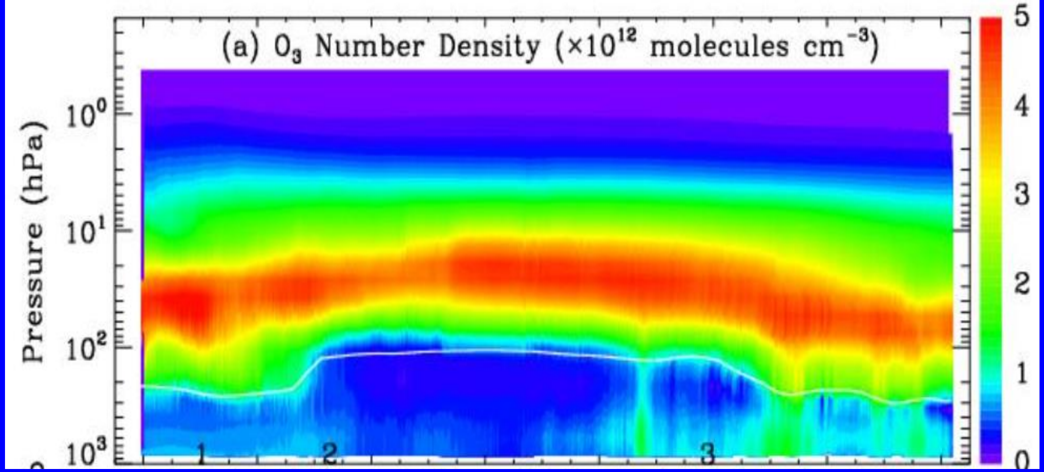
OMI Ozone Profile & Tropospheric Ozone Product (OMPROFOZ)

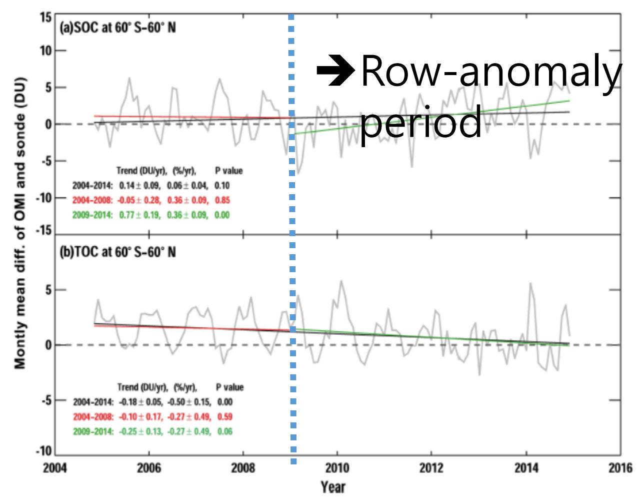
- **Liu et al. (2010)** : OMI ozone profiles from surface to ~65 km at 24 layers (3-7 layers in the troposphere) with **optimal estimation.** Tropospheric ozone column can be directly integrated.
- OMPROFOZ V1: OMI research ozone profile product, archived at AURA validation data center.





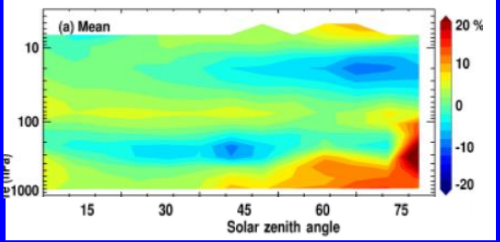
- **Validation efforts** : Huang et al. (2017;2008) over the OMI mission using ozonesonde and MLS found the long-term and spatial inconsistency of data quality.

❖ Trend Errors

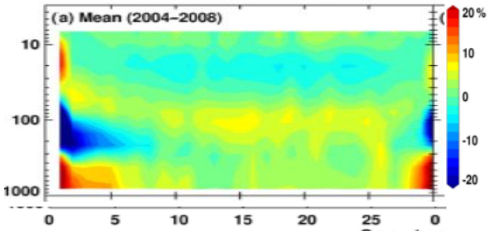


➔Row-anomaly period

❖ SZA-dependent Errors



❖ Cross track-dependent Errors



Updates for V2.0 OMPROFOZ

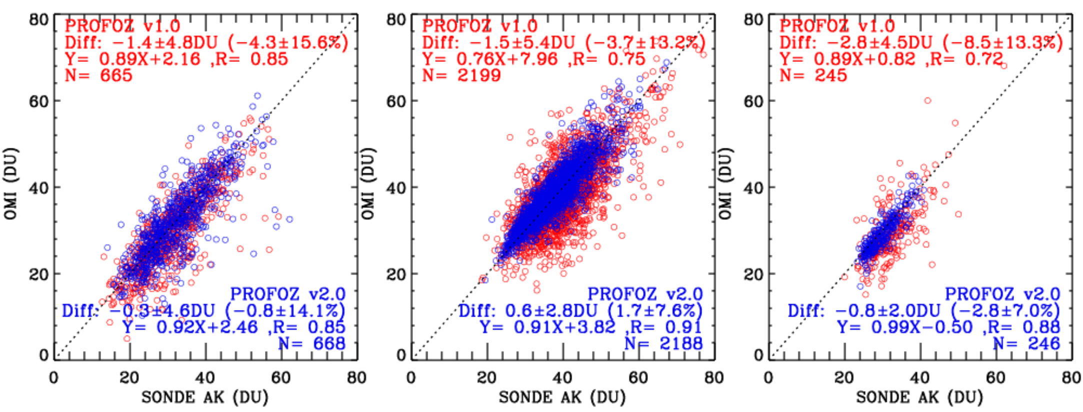
- Improve the retrieval accuracy and long-term consistency

implementations	V1.0	V2.0
1. A priori O3 data	Latitude/longitude dependent profile	Tropopause-dependent (TB) ozone profile
2. Meteorological data	NCEP/FNL model	NASA GEOS-5 model
3. Instrument Line Shape	Gaussian parameterization	Super Gaussian linearization
4. Irradiance	OMI 4-year mean spectra	OMI 31-day running mean spectra
5. Empirical calibration	2006m0711.dat	YYYYm0711-17.dat Common mode correction

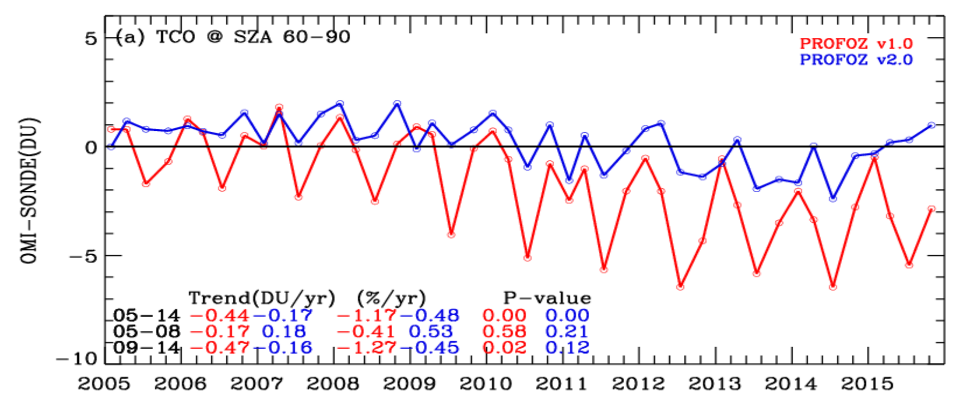
- Speed up radiative transfer calculation by a factor of ~4 and improve its accuracy
  - 2-half stream fast PCA-VLIDORT
  - Look-up table (LUT) correction of scalar vs. vector, 2. vs. 6 half streams, and ~24 vs. 48 layers

Updates for V2.0 OMPROFOZ

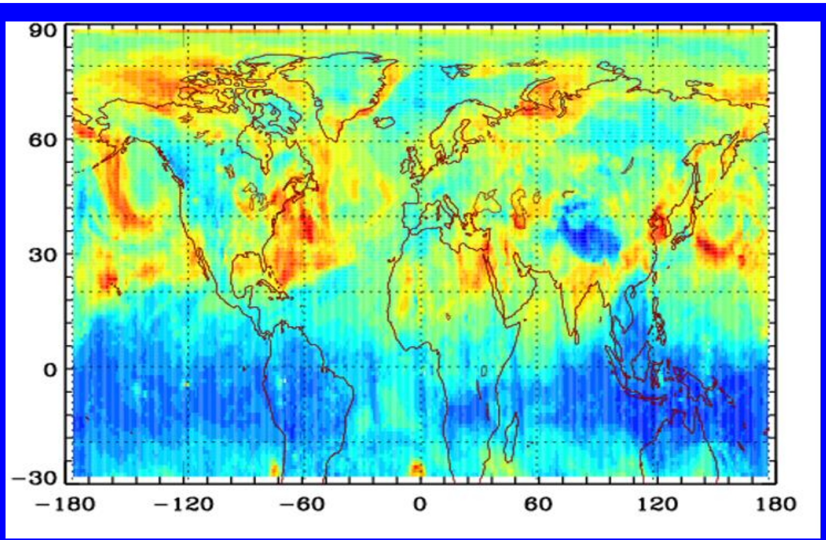
- Retrieval Accuracy → improved

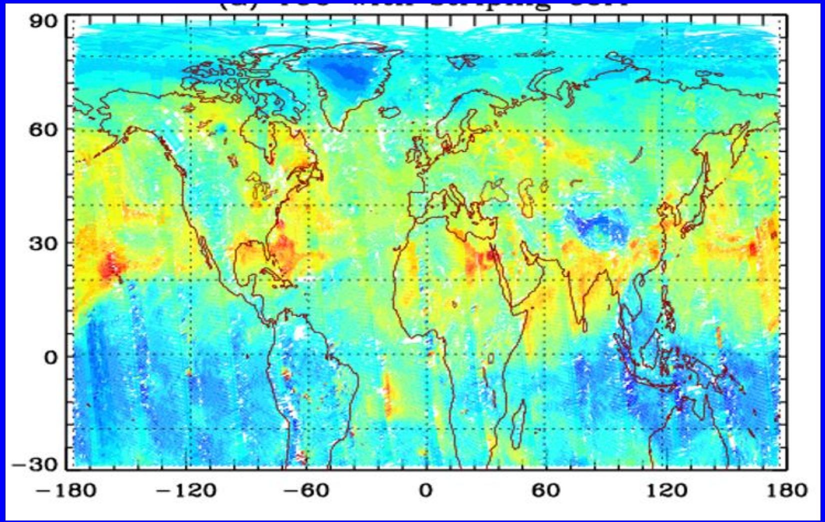


- Long-term consistency → improved



V1



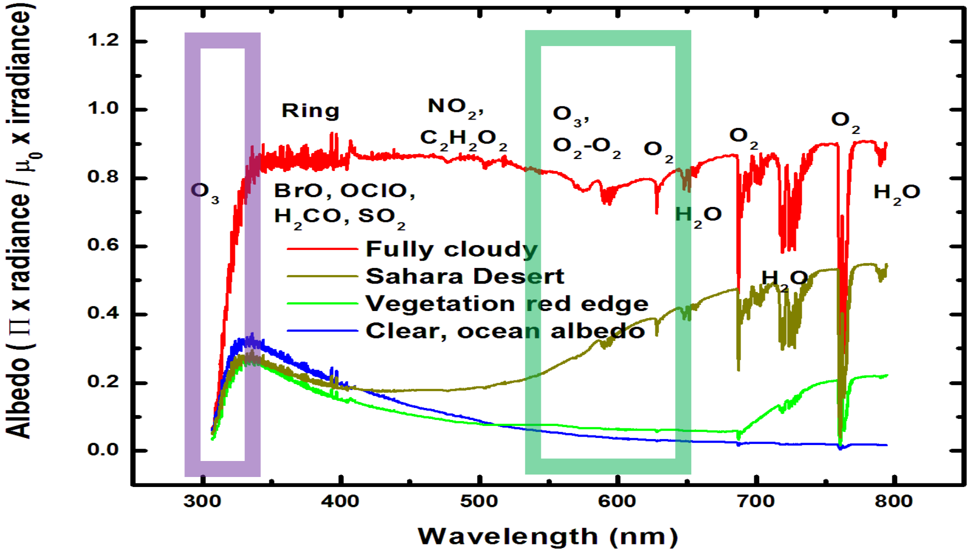


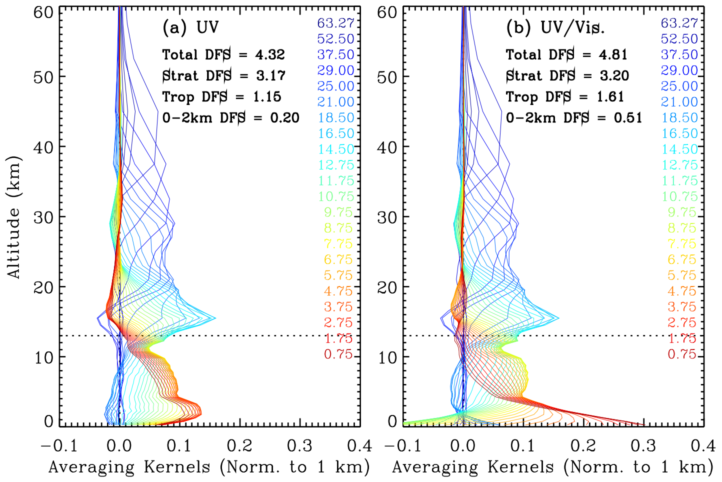
V2

- Improved implementations will be transferred into the OMI SIPS for routine processing of OMPROFOZ V2.0 soon.

TEMPO Joint UV/VIS Retrievals

- **UV (290-340 nm) & VIS(540-650 nm), @0.6 nm, 0.2nm/pixel**





❖ ***Benefits of visible fitting (Natraj et al., 2011; Zoogman et al., 2017)***

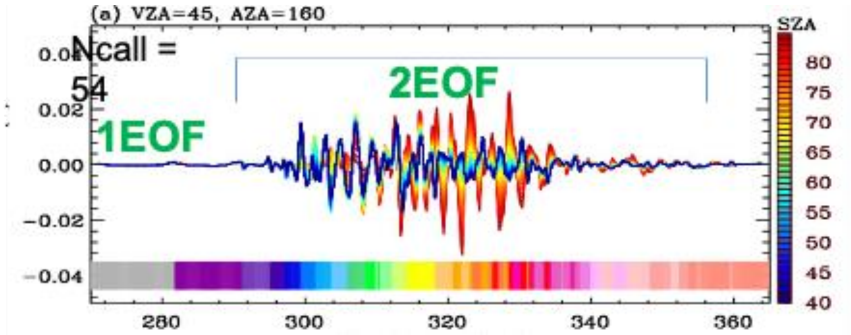
- UV + visible to help distinguish boundary layer O_3 from free tropospheric O_3.

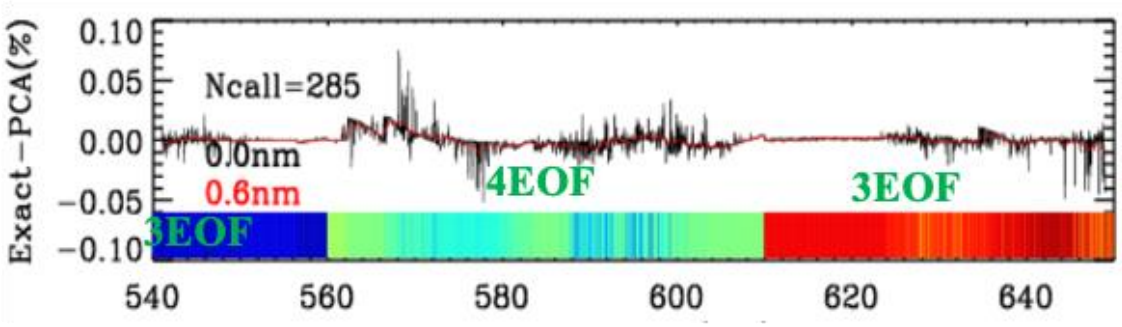
❖ ***Challenges of visible fitting***

1. Weak O_3 absorption, strong interferences from surface reflectance and aerosols/clouds, other gases (O_4, O_2, H_2O)
2. Need accurate radiometric calibration across the spectral range
3. Expensive RTM calculations at ∼800 wavelengths (with line-by-line calculations as fine as 0.002 nm in the visible)

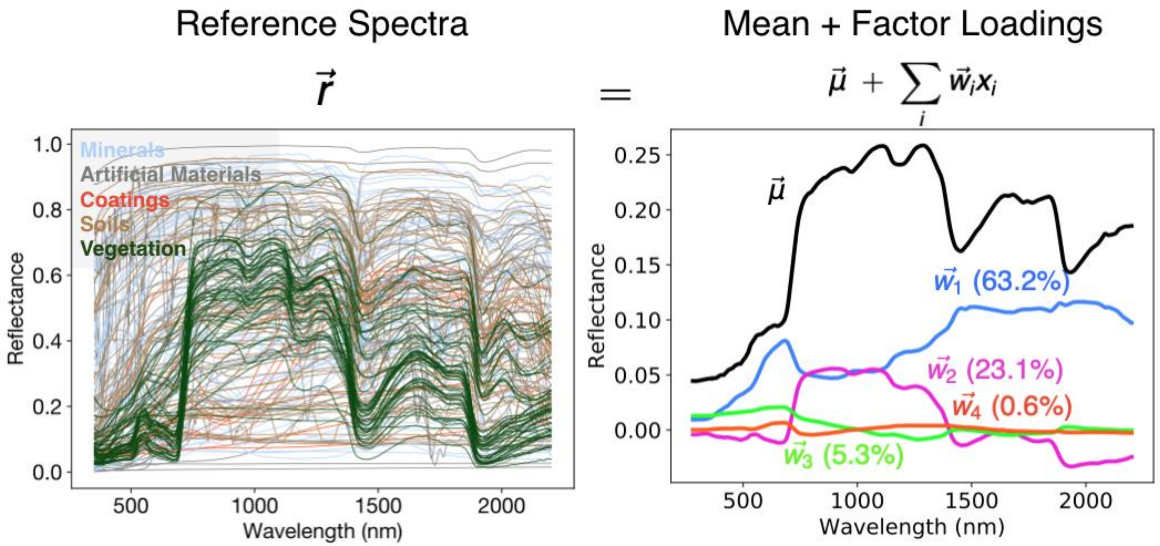
TEMPO Tropospheric O_3 Algorithm Status and Future Plan

- Adapted for TEMPO (with 0-2 km tropospheric O_3)
- HITRAN 2016 for O_2, H_2O (T & P) & O_4 (T) by Thalman et al. (2013)
- Implemented PCA-VLIDORT+LUT for UV/VIS: still need to account for H_2O and further speed up



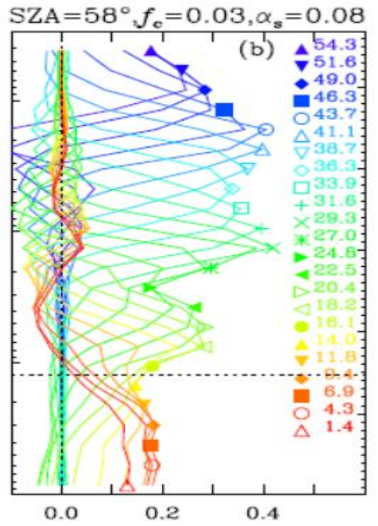


- Developed climatology of surface albedo spectra combining albedo spectra (ASTER + USGS + SCIAMACHY + other) + high spatial resolution MODIS albedo/BRDF for modeling the visible: still needs to be improved
- Merged ozone profile climatology (for OMI) with diurnally- resolved climatology in the troposphere (GEOS-5 nature run): GEOS-CF
- Account for aerosols and BRDF?



Back-up

1. A priori ozone information



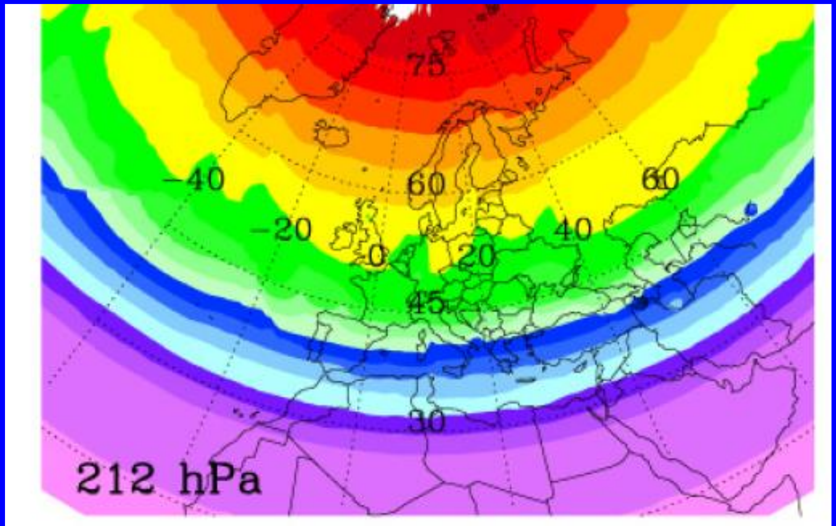
- ❖ $\hat{X} = X_{true} A + X_a (1 - A) + \varepsilon$

  X_a : A priori ozone information from climatological dataset.

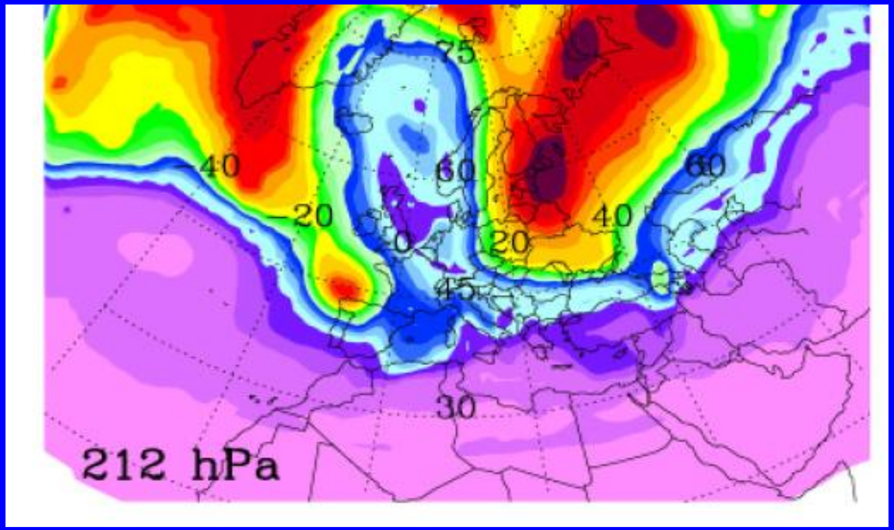
  A : sensitivity of measurements to the true atmospheric variability

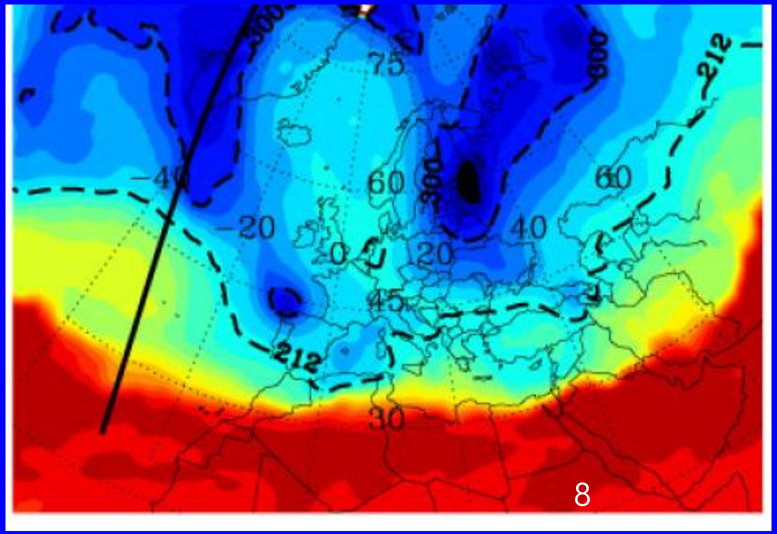
  $\hat{X} \Rightarrow X_a \; if \; A = 0$
- ❖ a typical nadir-BUV (Backscattered UltraViolet) instrument provides Insufficient vertical information on boundary layer and tropopause.
- ❖ Bak et al. (2013): constraint the ozone profile shape using the tropopause height.

■ **V1: Zonal mean climatology**



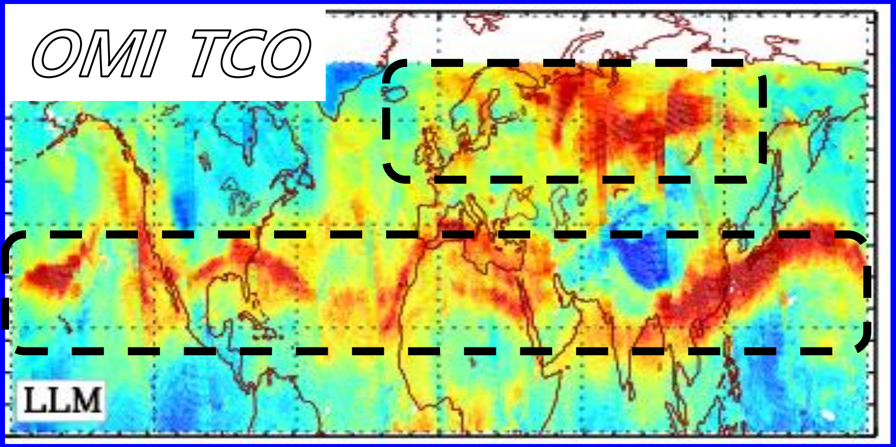
■ **V2: Tropopaused-based (TB) climatology**

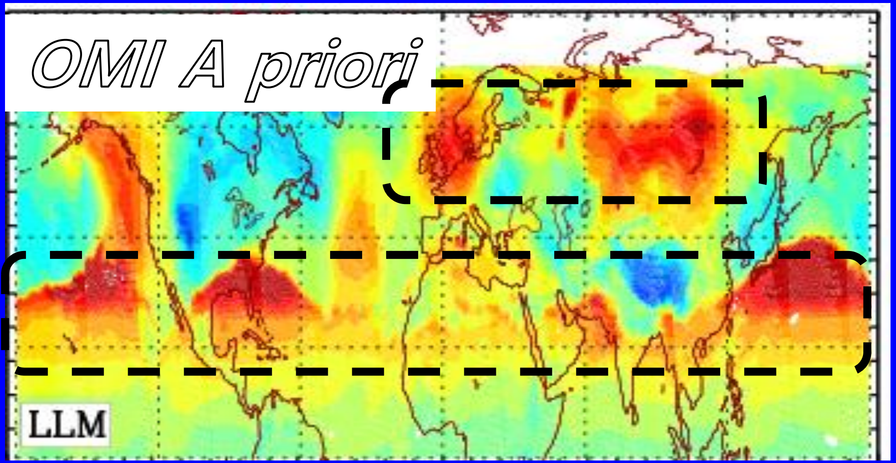




Example of different a priori on TCO retrievals (2007m0201)

🟥 V1: Latitude dependency



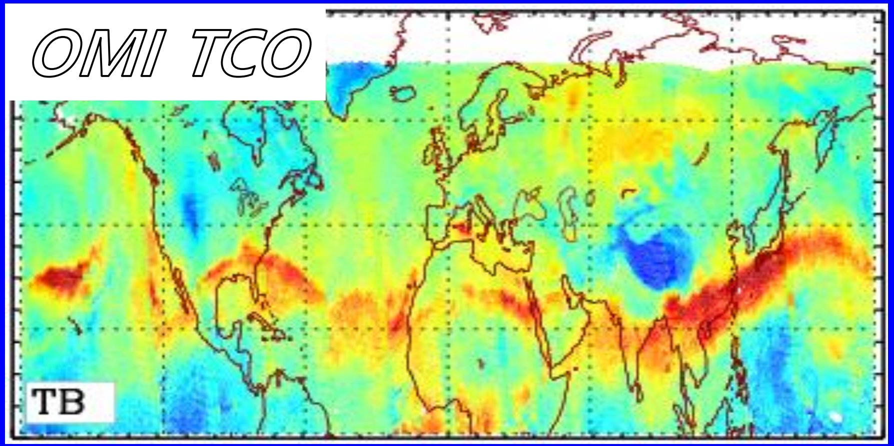


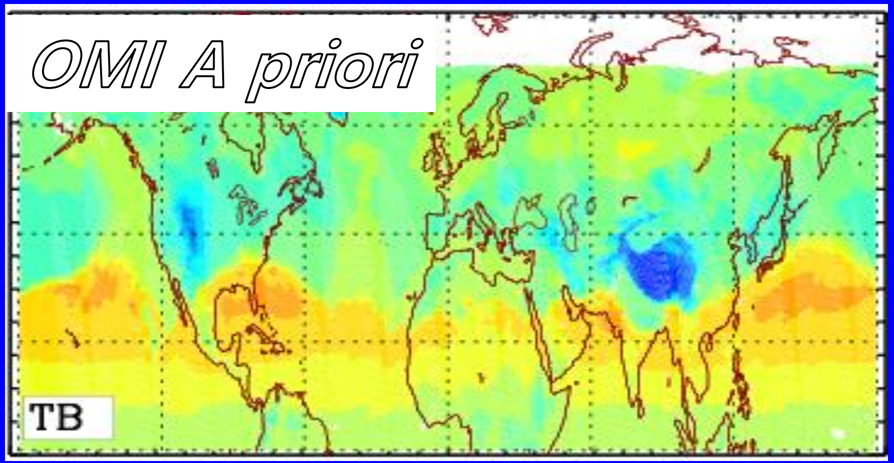
2007m0201

wrong a priori Information +
Less measurement information

wrong a priori Information +
some measurement information

🟥 V2: Tropopause-height dependency





2. Meteorological input

❖ **Surface pressure, tropopause pressure, temperature profiles**

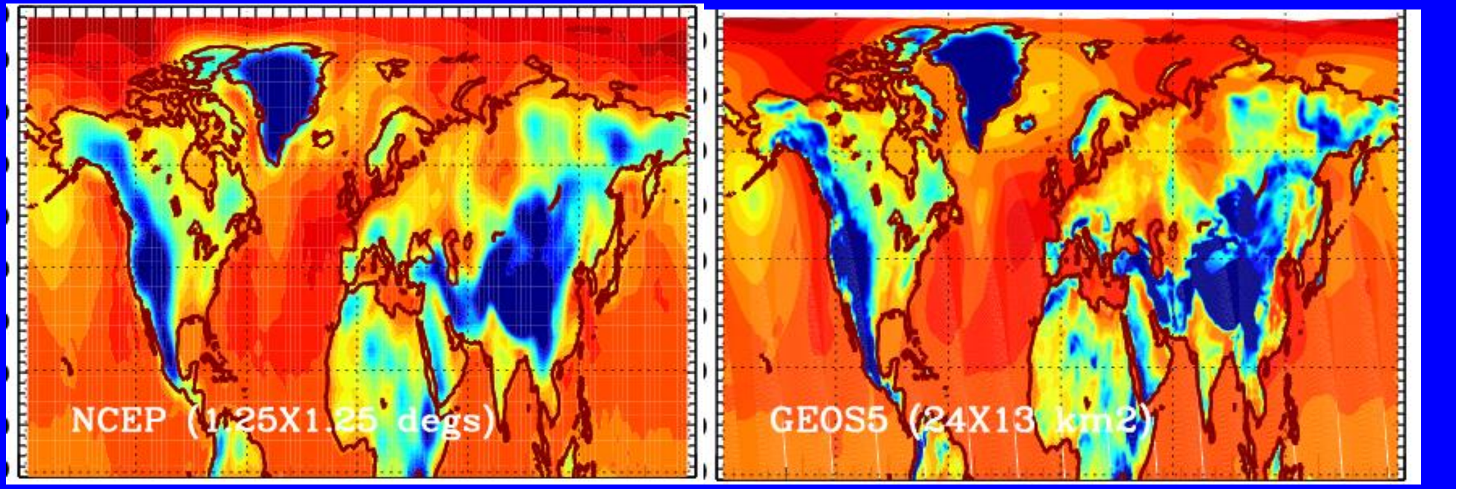
V1: NCEP (external)

- 6 hourly, 2.5 x 2.5 degree
- 17 levels up to 1 hPa

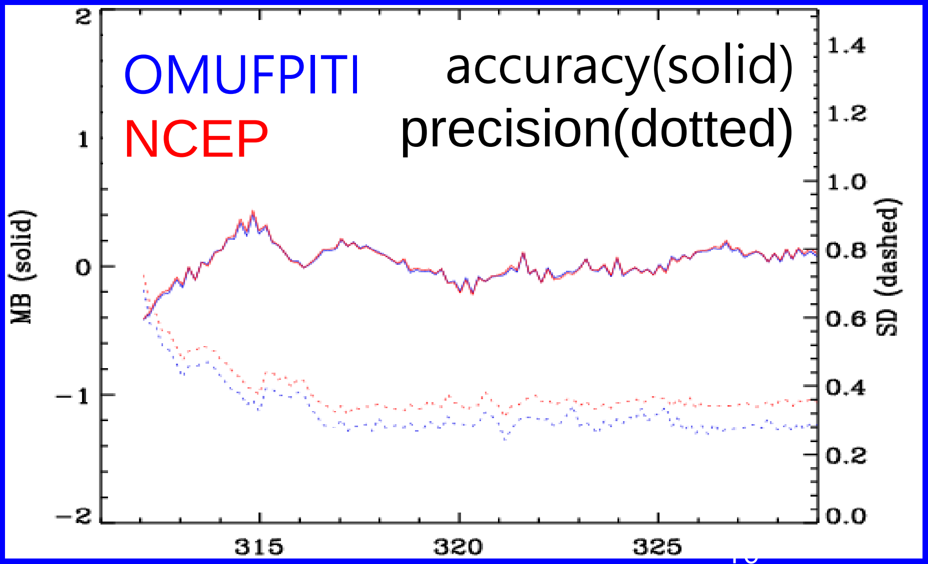
V2: OMUFPITMET (internal)

- GEOS5 model collocated to OMI time/UV2 spatial resolution (24 x 13 km2).
- 48 levels up to 1 hPa

❖ *surface pressure map comparison (hPa)*



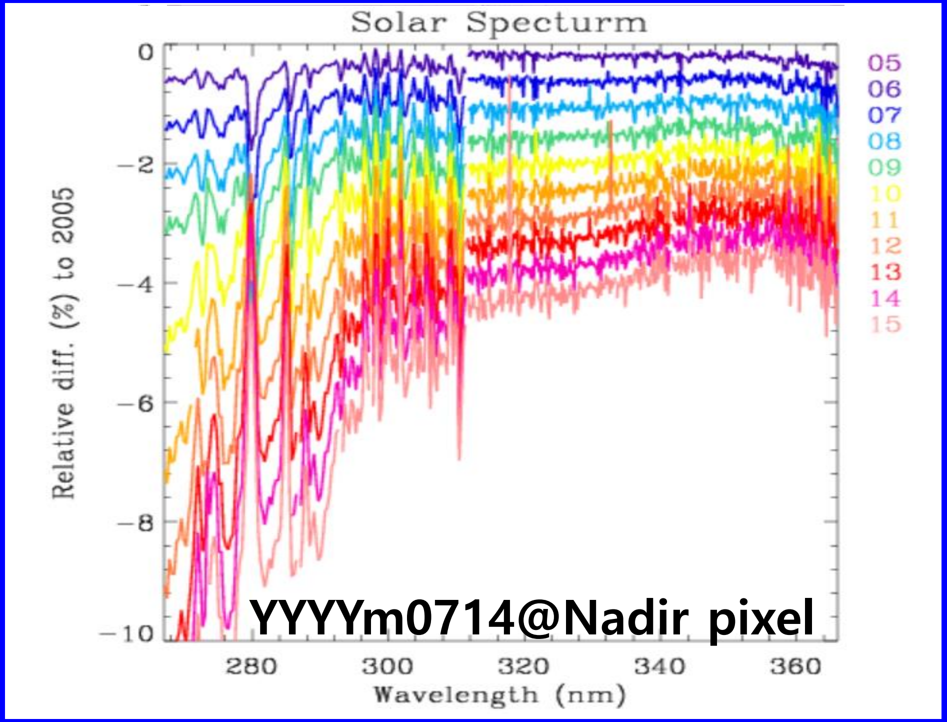
❖ *Impact on the fitting residuals*



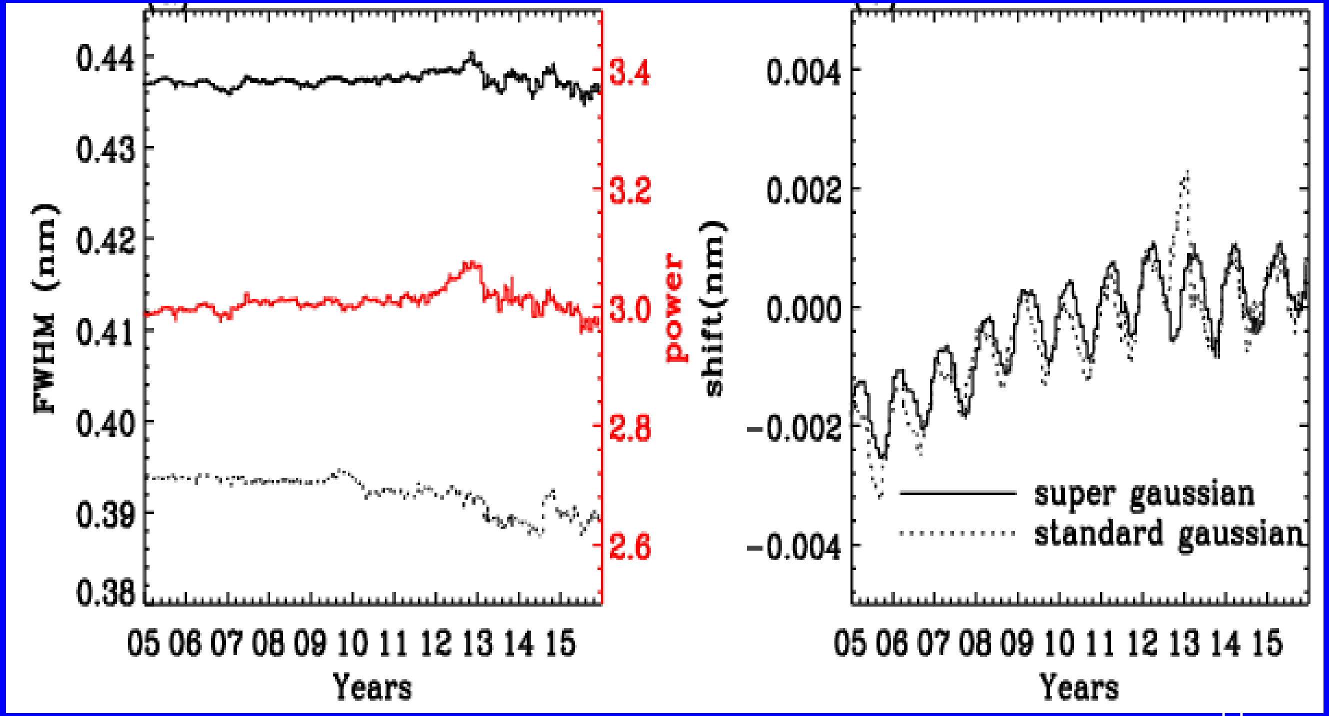
3. OMI irradiance

- OMI climatological irradiance spectra [2005-2007], to calculate normalized radiance and to estimate an on-orbit slit functions in PROFOZ v1.0, is switched to OMI 2-month running average in PROFOZ v2.0 for canceling out the degradation errors commonly existing in radiance and irradiance measurements.

(a) Relative change of irradiance from 2005



(b) Relative change of shift. /shift parameters from 2005

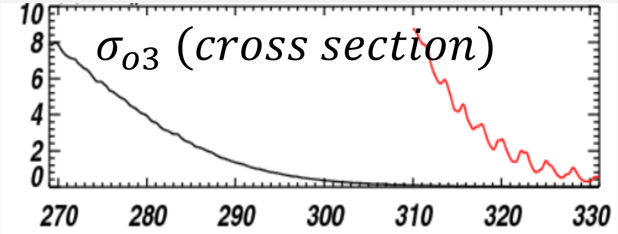


4. Instrument slit function

V1

- **Parameterized as Gaussian from irradiance**

$$G(X) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2}$$

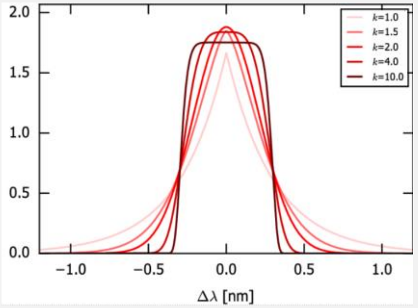

σ_{o3} (*cross section*)

V2

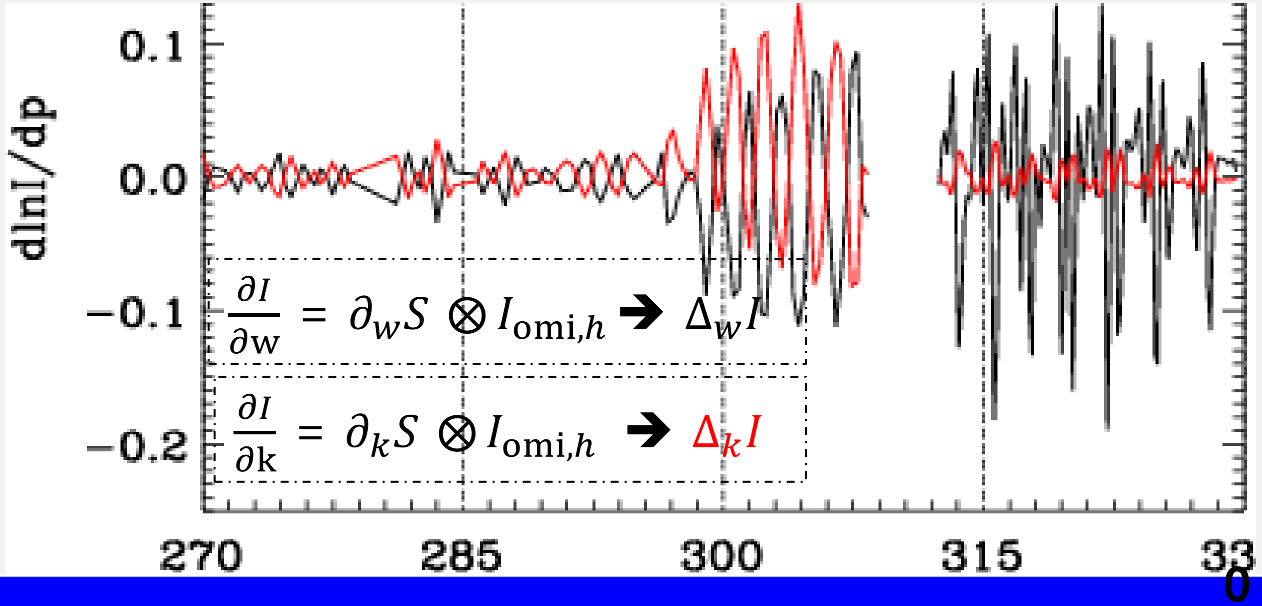
- **Parameterized as Super Gaussian from irradiance**

$$S(X) = \frac{k}{2\omega\Gamma(\frac{1}{k})} e^{-\left(\frac{x}{\omega}\right)^k}$$

K = shape factor, w= slit width



- **Linearize the effect of slit function errors on radiance fit : $\Delta_P I$ (Beirle et al., 2017; Bak et al. 2019)**

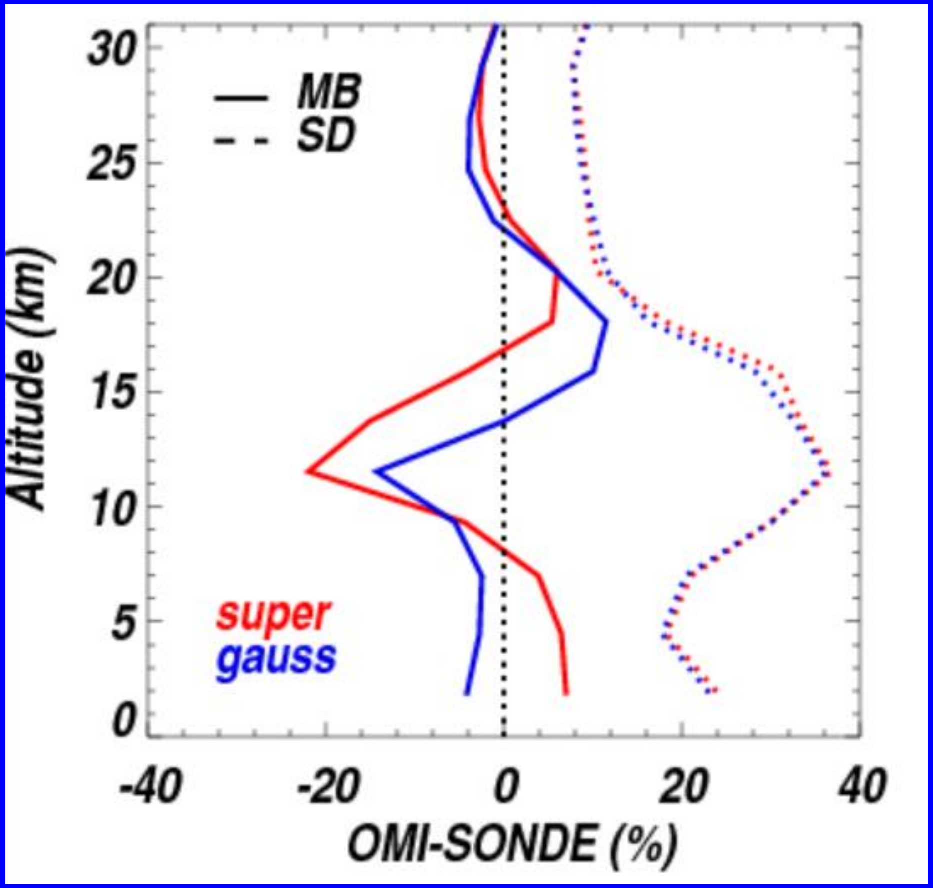


$$\frac{\partial I}{\partial \mathrm{w}} = \partial_w S \otimes I_{\mathrm{omi},h} \rightarrow \Delta_w I$$

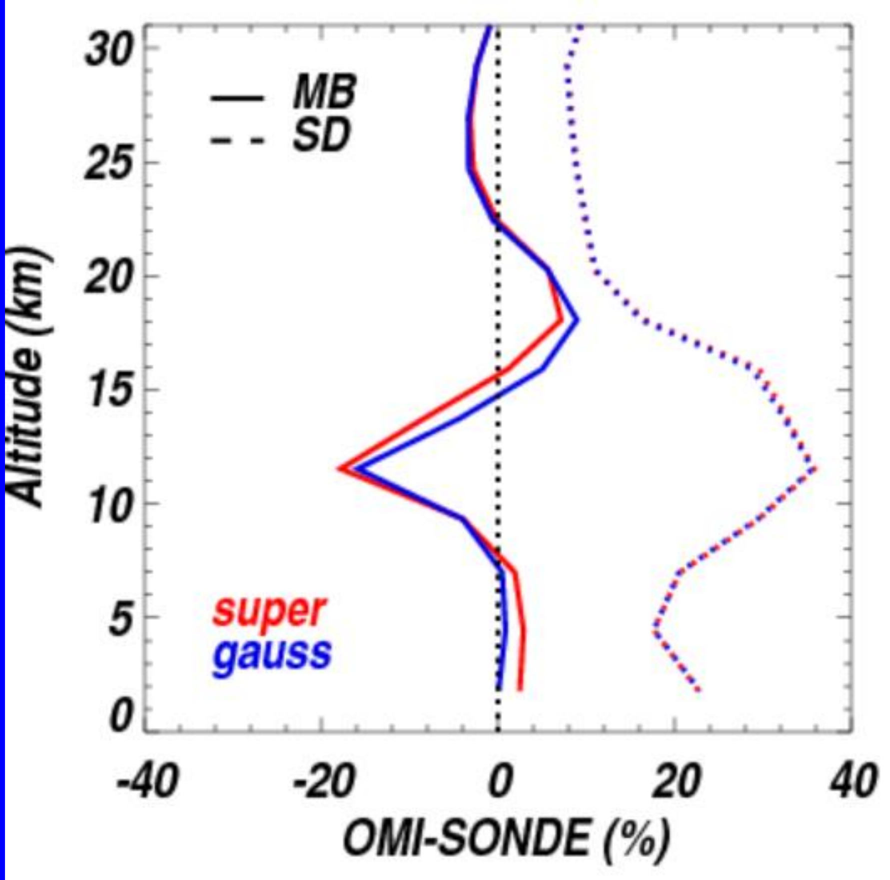
$$\frac{\partial I}{\partial \mathrm{k}} = \partial_k S \otimes I_{\mathrm{omi},h} \rightarrow \Delta_k I$$

OMI – SONDE (2005-2008)

- Without

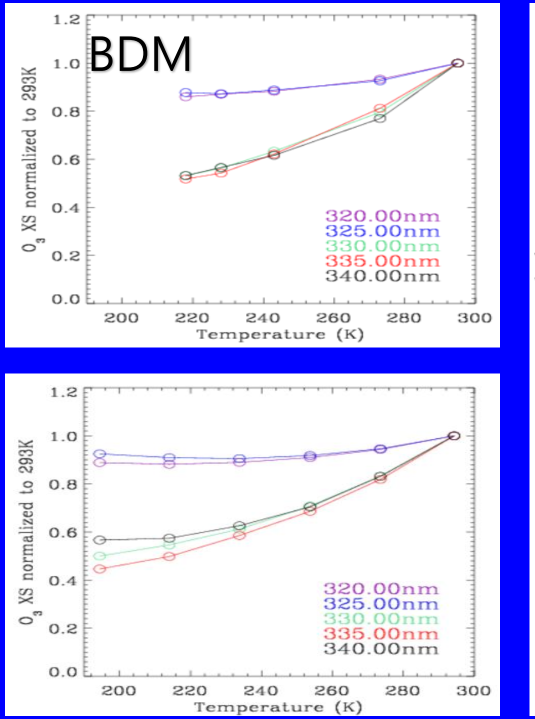


- With slit function error correction

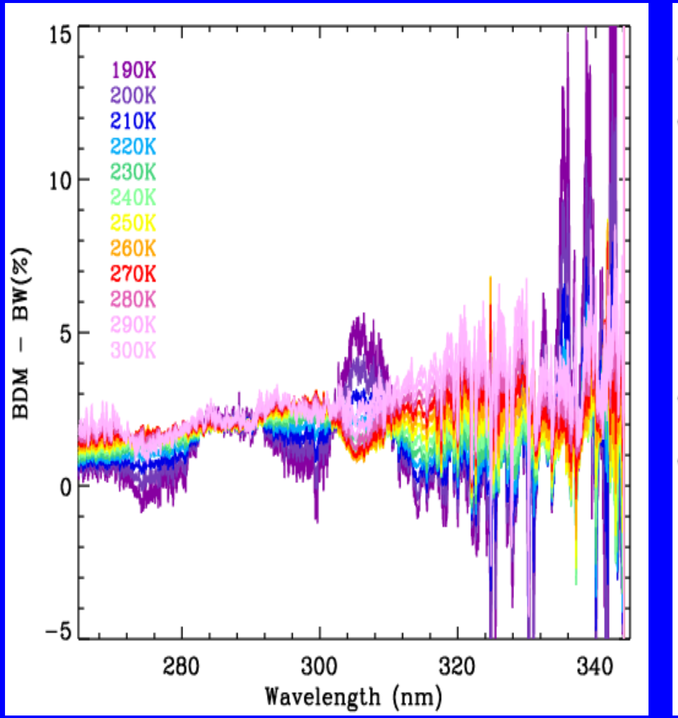


5. O3 cross-sections (BDM→ BW)

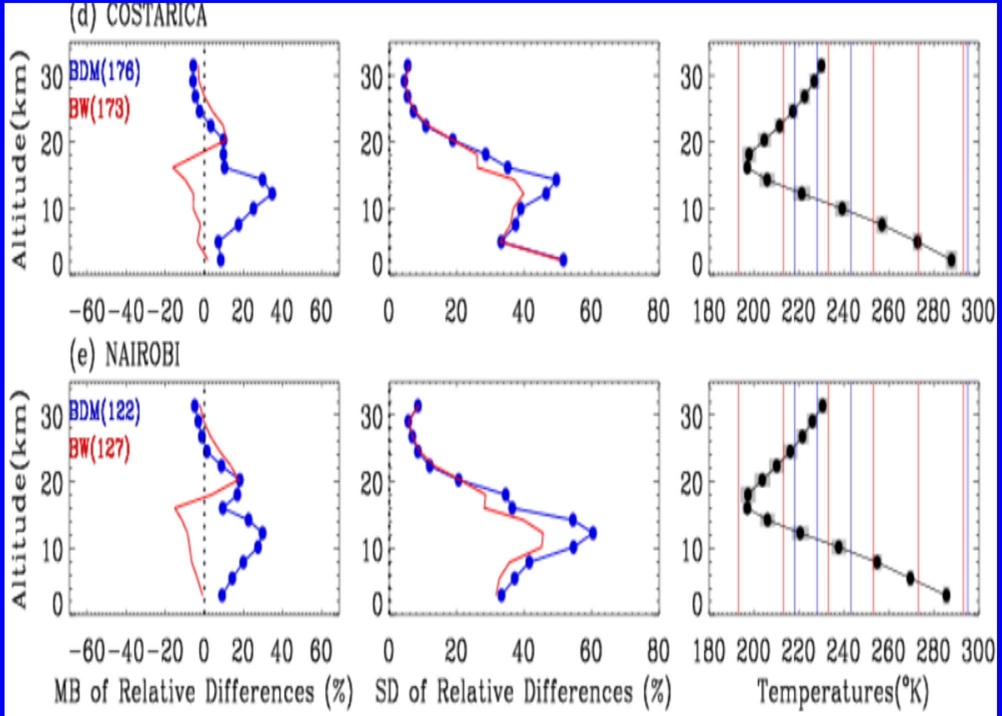
O3 CS (%)



BDM-BW (%)



OMI-SONDE (%)

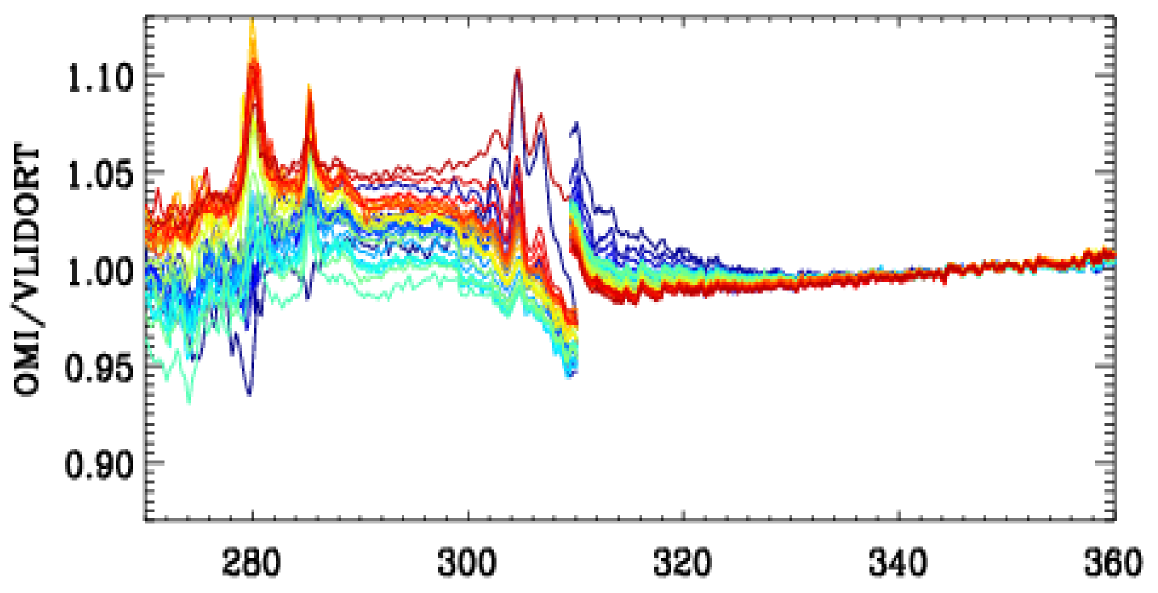


- **Brion-Daumont-Malicet (BDM) (1993)** : Current recommendation for ozone profile retrievals and column ozone over Bass and Paur (1985), and Serdyuchenko et al (2016) in Liu et al. (2007) and Liu et al. (2013)
- **Birk and Wagner (13NOV2018)** : at the German Aerospace Center (DLR) within the framework of the ESA project in order to improve the atmospheric BUV retrievals from the TROPOMI instrument

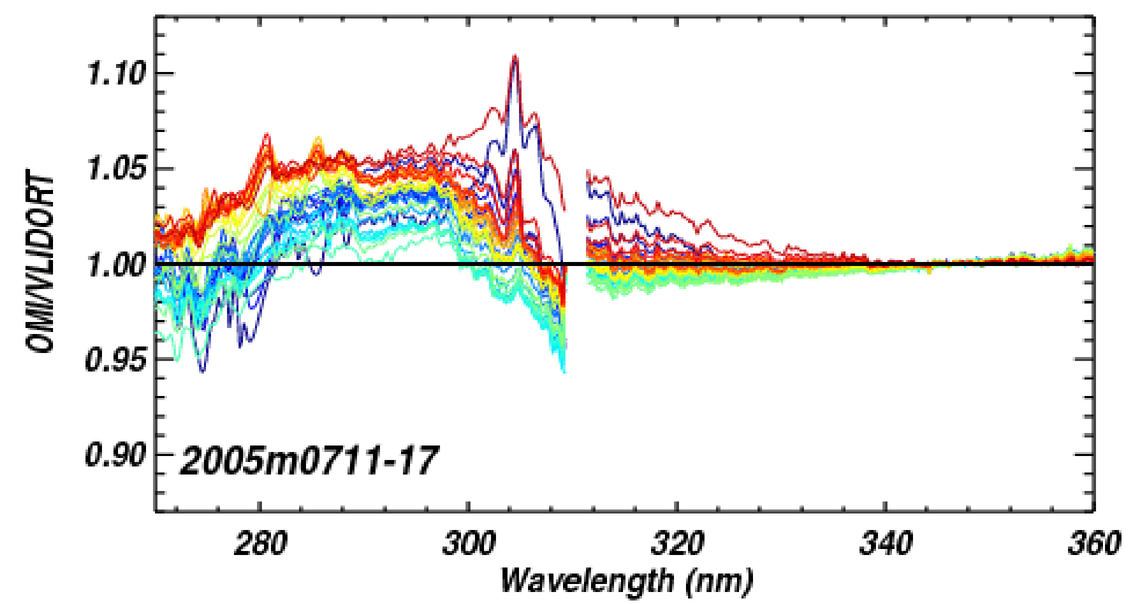
5.1 Soft Calibration

- kind of systematic differences of $I_{OMI} - I_{RTM}$ characterized as a function of cross-track and wavelengths using one day of tropical cloud-free measurements

V1: 2006m0711.dat



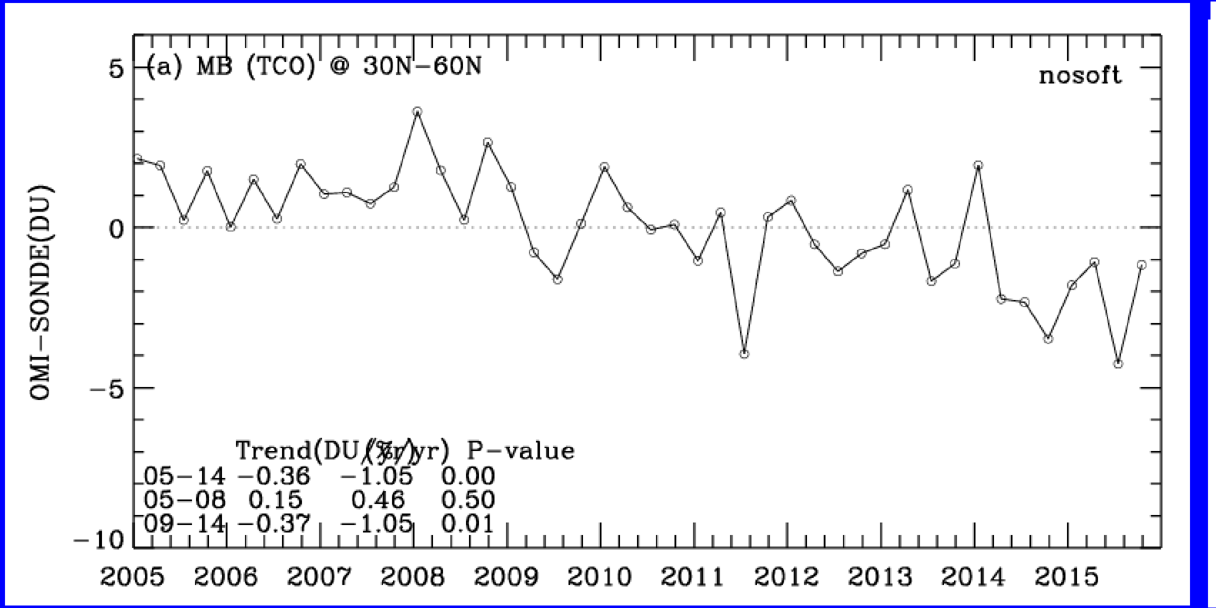
V2: YYYYm0711-17.dat

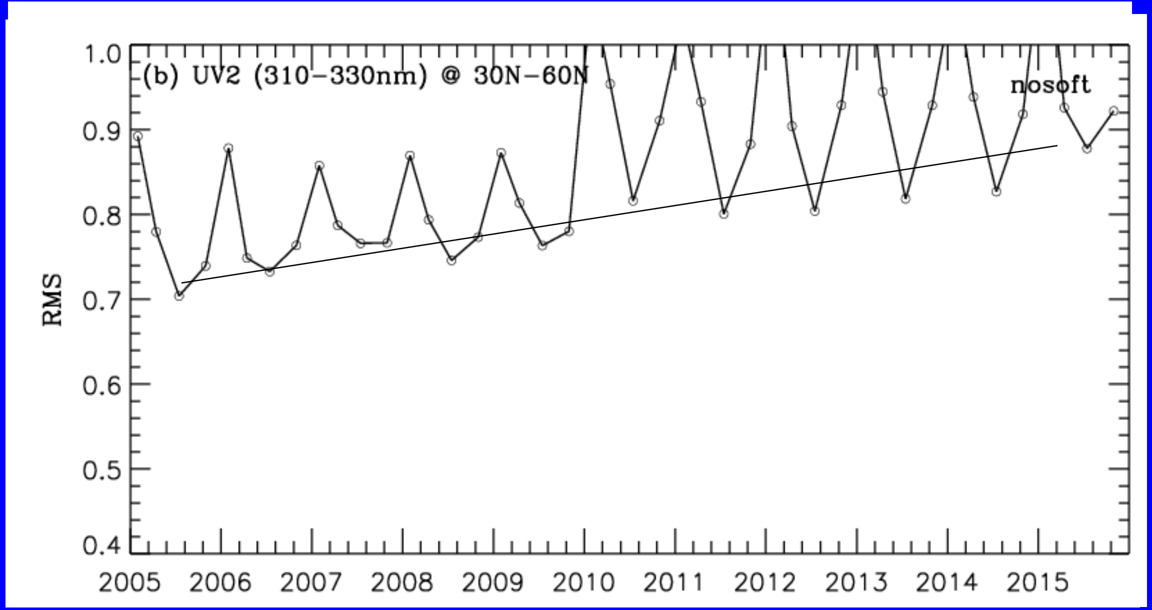


Evaluation of soft calibration implementation

■ **Time-series : TCO (OMI-SONDE)**

■ **RMS of UV2 fitting residuals(310-330 nm)**

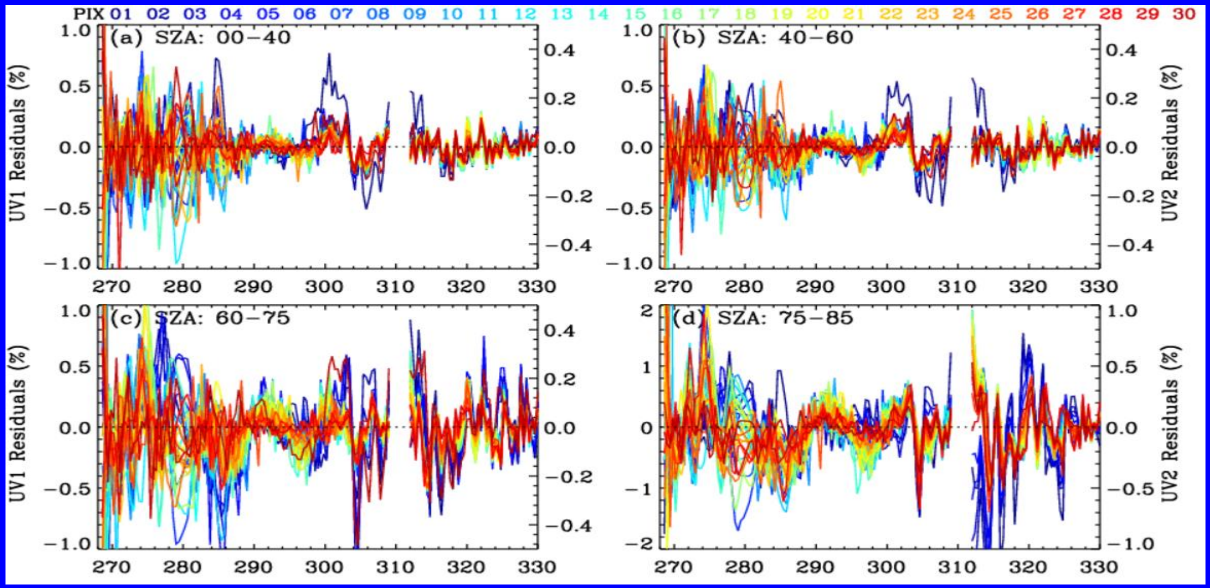




- **No soft calibration**
  - Inconsistency of TCO errors as of 2008 and linear degradation of Fit. accuracy.
- **Old soft calibration (2006)**
  - Reduction of systematic biases of both TCO and Fit residuals.
- **New soft calibration (YYYY)**
  - Reduction of seasonal biases due to improvements of TCO retrieval errors and Fit. accuracy in summer.

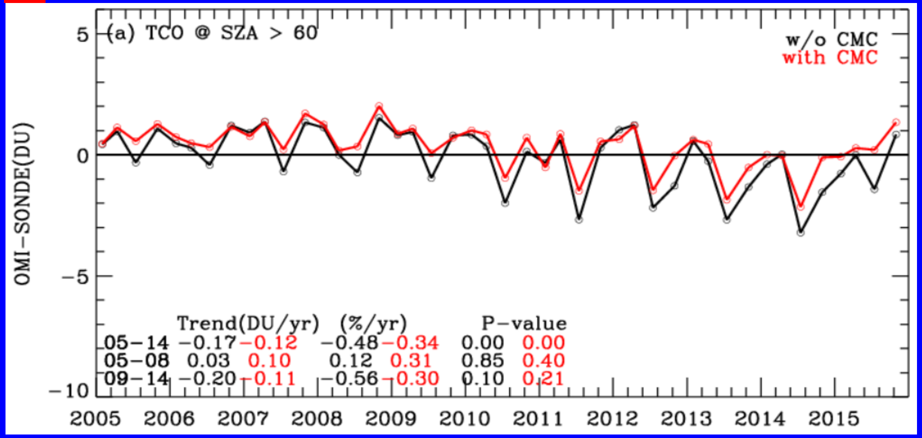
5.2 Common mode correction (CMC)

- In order to compensate the soft calibration, especially out of tropics, remaining residuals after soft calibration is characterized as <u>a function of Lambda, cross-track</u>, and solar zenith angle for each month.

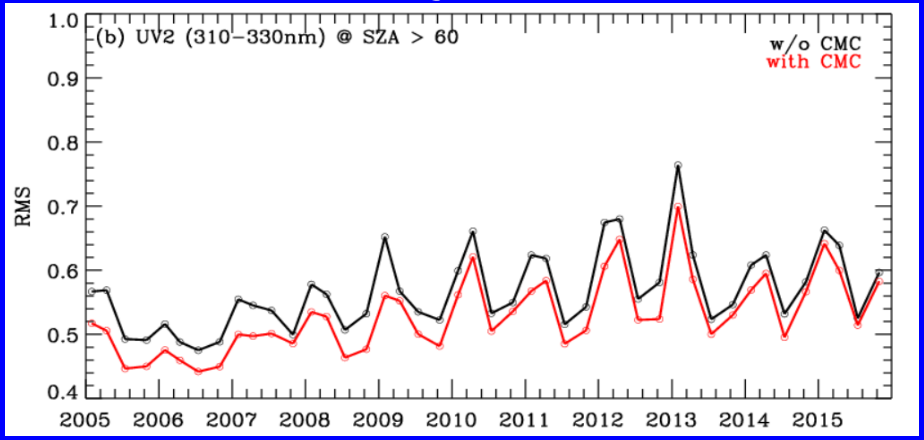


- applied as a pseudo absorber. The amplitude of correction spectrum is iteratively adjusted with the corresponding coefficient in term of a state vector.

■ OMI-SONDE TCO



■ RMS of Fitting Residuals in UV2



6. Radiative Transfer (RT) model

- **OMI wavelengths: 270-310 nm @ 0.33nm/pxl, 310-330 nm @ 0.14nm/pxl ➔ $\lambda_n = 208$**
- **OMPROF (SAO) : 4 pixel co-adding due to limitation of computational budget.**

v1	▪ **VLIDORT v2.4 model** a. on-line 4 stream scalar calculation at effective ***78*** λ_e (1.0nm at $\lambda_\mathrm{h} < 290$, 0.4nm, 0.6nm at $> 310\mathrm{nm}$) b. on-line polarization correction at selected **11** λ c. interpolation onto $\lambda_\mathrm{h}(= 0.05\mathrm{nm})$ with its error correction based on differences in optical properties at λ_e and λ_h :$I = I + \frac{dI}{dtau}\,(\tau_h - \tau_e)$ d. interpolation and convolution onto λ_{OMI}
V2	▪ **PCA (principal component analysis)-VLIDORT** a. online 2 stream scalar calculation at $\lambda_\mathrm{h}(= 0.05\mathrm{nm})$ $N\lambda_{\mathrm{vlidot}}(slow\ accurate\ MS) = \mathbf{54}, N\lambda_{2st}(fast\ accurate\ SS) = \mathbf{1160}, N\lambda_{\mathrm{FO}} = 1160(fast\ approx\ MS)$ **➔ computational cost is reduced due to less VLIDORT calls (78➔ 54, 1.45 times) and use of less nstream (4→2, 4 times)** b. **LUT correction** for RTM errors arising from vector vs. scalar and 6 vs 2 stream, **48** vs 24 layers c. interpolation and convolution onto λ_{OMI}

6. Radiative Transfer (RT) model

- **OMI wavelengths: 270-310 nm @ 0.33nm/pxl, 310-330 nm @ 0.14nm/pxl ➔ $\lambda_n = 208$**
- **OMPROF (SAO) : 4 pixel co-adding due to limitation of computational budget.**

CALL **VLIDORT v2.4 ➔** I_s

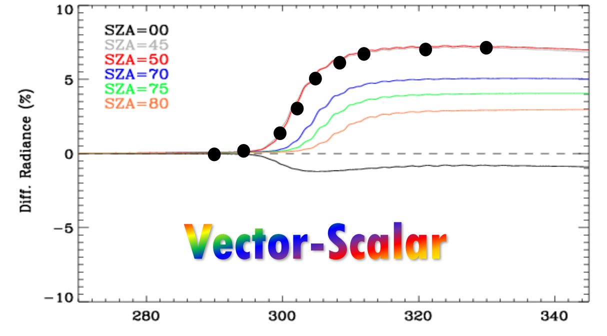
4stream scalar at 78 λ_e

(1.0nm at $\lambda_\mathrm{h} < 290$, 0.4nm, 0.6nm at > 310nm)

$$I = I_s + \Delta C_{on-line}$$

CALL VLIDORT in vector At **11** λ

$$\Delta C_{on-line} = \Delta(vec\ - sca)$$



Interpolation/correction @ 0.05 nm (N=1160)

$$I(\lambda_h) = I(\lambda_c) + \frac{\partial I\ (\lambda_c)}{\partial \Delta_l^{gas}}\ \left(\Delta_l^{gas}(\lambda_h) - \Delta_l^{gas}(\lambda_c)\right) + \frac{\partial I\ (\lambda_c)}{\partial \Delta_l^{ray}}(\Delta_l^{ray}(\lambda_h) - \Delta_l^{ray}(\lambda_c))$$

Convolution/interpolation

@ OMI grids (N=208)
in 270-330 nm

6. Radiative Transfer (RT) model

- **PCA(Principal Component Analysis)-VLIDORT RT (Spurr and Natraj et al., 2013) : reducing the time-consuming multiple scattering calculation after grouping individual wavelengths into several bins based on optical properties.**

CALL **PCA VLIDORT** ➔ I_s

2stream scalar at 0.05 nm

(N= 1160)

$$I = I_s + \Delta C_{LUT}$$

$$\Delta C_{LUT} = \Delta(vec - sca) + \Delta(6str - 2str) + \Delta(48layer - 24layer)$$

Convolution/interpolation

@ OMI grids (N=208)

in 270-330 nm