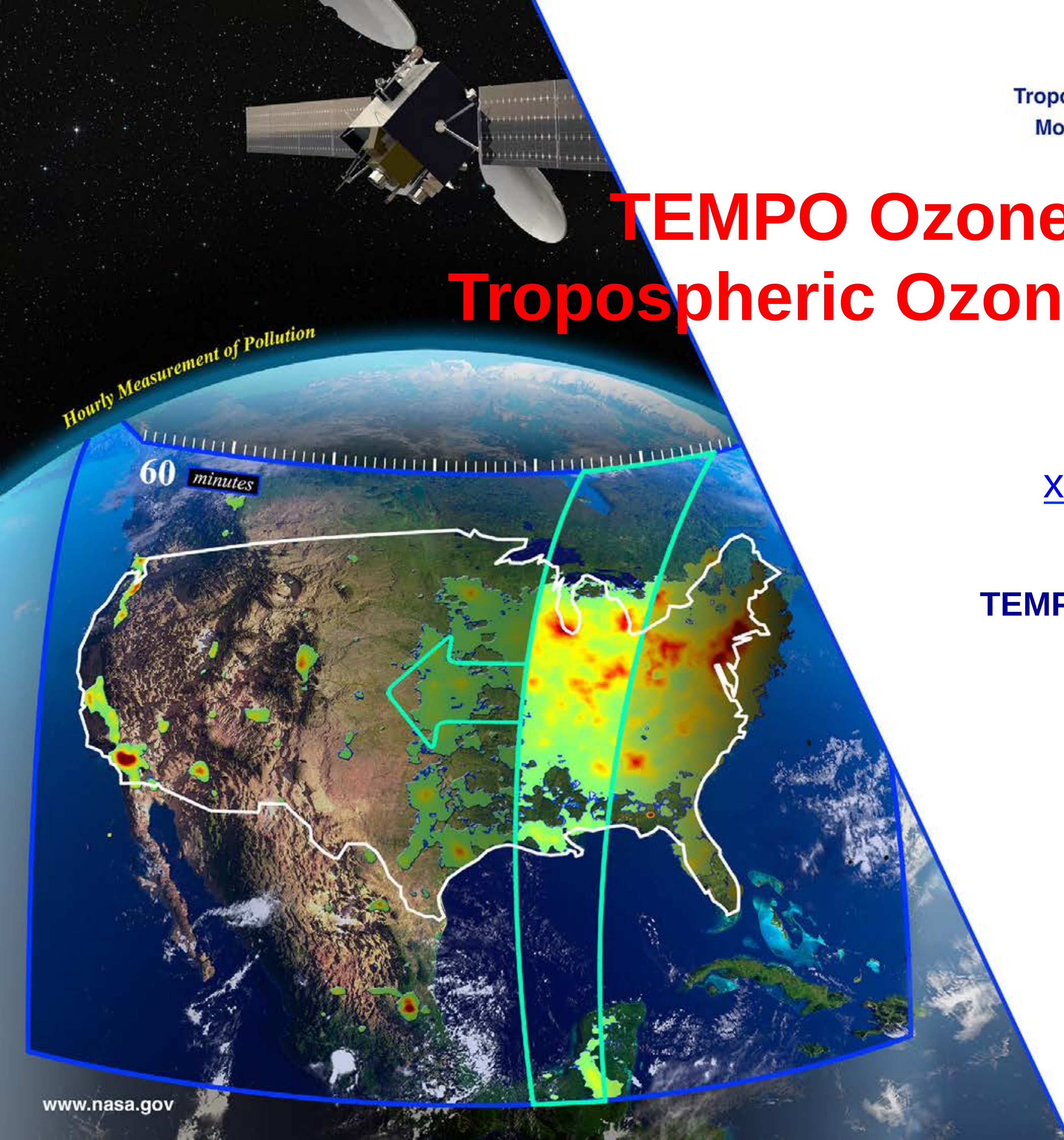
Tropospheric Emissions: Monitoring of Pollution

TEMPO

TEMPO Ozone Profile and Tropospheric Ozone Retrievals



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TEMPO Validation Workshop

Berkeley, CA

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Smithsonian

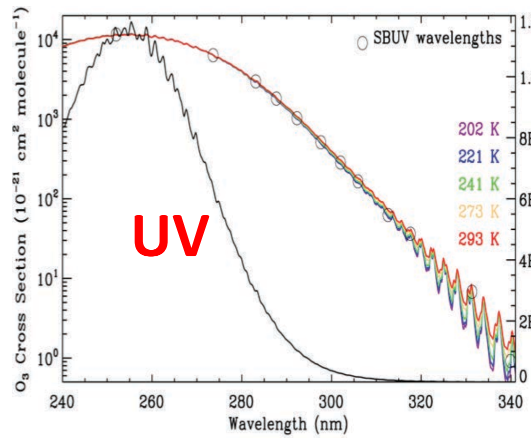
NASA

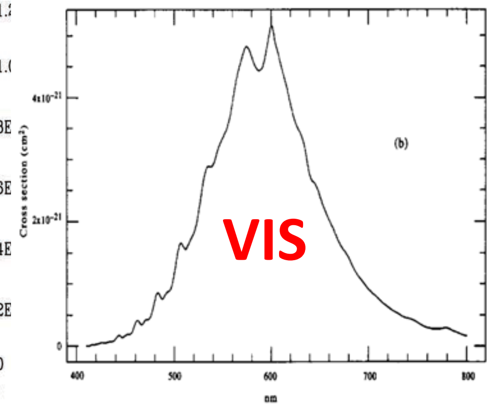
Outline

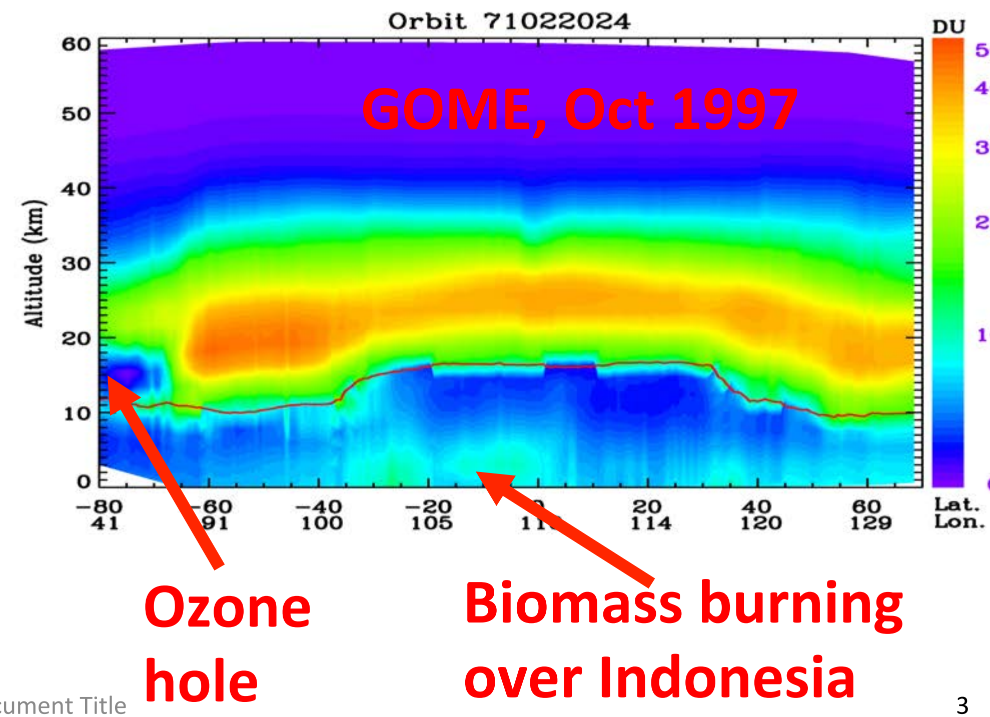
- Introduction
- OMI Ozone Profile Retrieval
- Validation of OMI Retrievals with Ozonesonde and MLS
- Adaption of OMI Algorithm for TEMPO
  - Perform synthetic UV/visible retrievals
  - UV/visible retrievals from GOME-2 data
- Summary and Future Outlook

Introduction

- **Chance et al. (1991, 1997): possible to retrieve ozone profile including tropospheric ozone from backscattered UV/Visible spectra.**
- **Demonstrated retrievals of tropospheric O_3 from GOME, GOME-2, OMI UV data by various groups (Munro et al., 1998; Hoogen et al., 1999; Hasekamp and Landgraf, 2001; van der A et al., 2002; Liu et al., 2005, 2010; Cai et al., 2012; van Peet et al., 2014; Miles et al., 2015).**
- **However, UV only retrievals provide limited retrieval sensitivity to lower tropospheric ozone.**

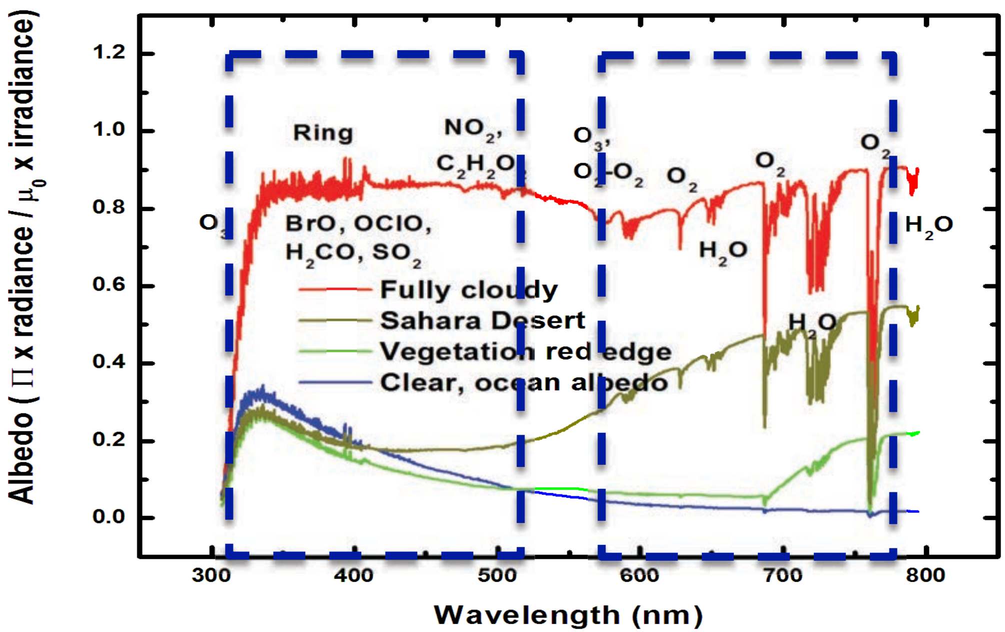


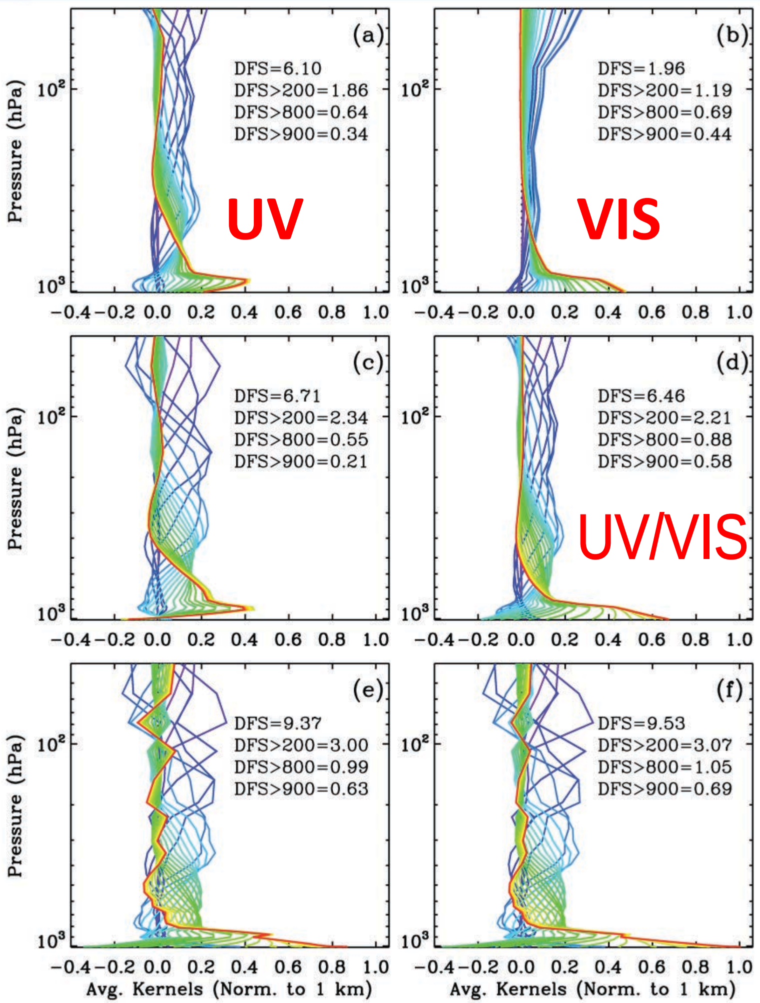




Introduction

- GEOCAPE multispectral sensitivity studies: combine UV with visible and/or TIR can greatly improve sensitivity to 0-2 km O_3 (Natraj, Liu et al., 2011).
- TEMPO: UV (Hartley/Huggins bands) + Visible (Chappuis bands) to distinguish boundary layer O_3 from free troposheric and stratospheric O_3





(a) UV (b) VIS (c) TIR (d) UV+VIS
(e) UV+TIR (f) UV+VIS+TIR

4

Introduction

- **Visible retrievals: shown to improve tropospheric O_3 column from SCIAMACHY data by neural network algorithms (Sellitto et al., 2012a,b).**
- **Challenges: weak visible O_3 absorption, strong interferences from surface reflectance and aerosols/clouds, consistent radiometric calibration across the spectral range**
- **We have used GOME-2 data to test this UV/visible approach. But GOME-2 are not ideal for testing this algorithm : peak of Chappuis bands is split into bands 3 and 4, radiometric calibration inconsistency**
  - 1a: 240-307/283* nm, 0.25 nm FWHM   * changed in December 2008
  - 1b: 307/283-315 nm, 0.25 nm FWHM
  - 2: 311-403 nm, 0.25 nm FWHM
  - 3: 401-600 nm, 0.5 nm FWHM
  - 4: 590-790 nm, 0.5 nm FWHM
- **UV/visible O_3 profile retrieval using physically based algorithm has yet to be demonstrated from real data.**
- **We identified this as an instrument project science risk for TEMPO.**

03 Instrument Project Science: Ozone Retrieval Performance

ID: 0003

Domain

Technical

L x C

2 x 3

Response

Mitigate

Given that TEMPO's technique of combining UV and visible radiances for retrieving lower tropospheric (0-2 km) O_3 concentration has never been validated using existing nadir satellite measurements, and that TEMPO will attempt to make such measurements at finer spatial resolution than previous satellites, there is a possibility that TEMPO may not achieve 10 ppbv precision for 0-2 km O_3 concentrations during Phase E, which can result in a degradation of the TEMPO Instrument baseline science performance for the lower tropospheric O_3 product but higher than threshold.

Response Plan Step	Start Date	End Date	Expected L x C
1) Develop wavelength-dependent and angle dependent surface albedo /BRDF) database at high spatial resolution over the TEMPO field of regard by combining MODIS albedo/BRDF product, ASTER spectral library and land cover types. COMPLETE	1/2014	11/2014	3 x 3
2) Perform non-linear ozone profile retrievals from simulated radiances, utilizing the developed albedo/BRDF database, and verify that the retrievals are self-consistent with the input profiles to within calculated retrieval uncertainties, to demonstrate the TEMPO approach can work theoretically for selected surface scenes. COMPLETE	1/2016	1/2016	2 x 3
3) Apply the developed Albedo/BRDF database to GOME-2 retrievals, and perform empirical radiometric calibrations to GOME-2 data to improve the consistency among Huggins bands and two parts of Chappuis bands in different channels, to demonstrate the TEMPO approach can work at coarse resolution and over various scenes. In process.	1/2014	6/2017	2 x 2
4) Assess the quality of ACAM/GEO-TASO data and demonstrate high spatial resolution combined UV/Visible ozone retrievals over a variety of scenes from ACAM and GEO-TASO aircraft measurements. In process (ACAM & GeoTASO measurements obtained during July-Aug deployment to Denver with DISCOVER-AQ have acquired the data for this response – progressing on schedule).	1/2014	9/2017	2 x 1
5) Use TEMPO as-built instrument characterization database and high spatial/spectral resolution reflectance database in retrieval simulations to verify expected on-orbit retrieval performance.	1/2016	2/2018	1 x 1

Risk Owner: Xiong Liu

SAO OMI Ozone Profile Retrieval Algorithm

- **Initial OMI algorithm (Liu et al., 2010): adapted from GOME**
  - **Spectral fitting + full radiative transfer simulation (VLIDORT)**
  - **Retrieve O_3 partial columns at 24 layers from surface to ~60 km, total, stratospheric, tropospheric ozone columns are integrated with the use of NCEP tropopause**
  - **Fitting windows: 270-309, 311-330 nm**
  - **3-year mean solar irradiance spectra + soft radiometric correction**
  - **Ill-posed problem: non-linear optimal estimation (Rodgers, 2000) with zonal mean O_3 profile climatology (McPeters et al., 2007)**

$$\chi^2 = \left\| \mathbf{S}_y^{-\frac{1}{2}} \{\mathbf{K}_i(\mathbf{X}_{i+1} - \mathbf{X}_i) - [\mathbf{Y} - \mathbf{R}(\mathbf{X}_i)]\} \right\|^2 + \left\| \mathbf{S}_a^{-\frac{1}{2}} (\mathbf{X}_{i+1} - \mathbf{X}_a) \right\|^2$$

$$\mathbf{X}_{i+1} = \mathbf{X}_i + (\mathbf{K}_i^T \mathbf{S}_y^{-1} \mathbf{K}_i + \mathbf{S}_a^{-1})^{-1} \{\mathbf{K}_i^T \mathbf{S}_y^{-1} [\mathbf{Y} - \mathbf{R}(\mathbf{X}_i)] - \mathbf{S}_a^{-1} (\mathbf{X}_i - \mathbf{X}_a)\}$$

Y: Measurement vector (e.g., radiances)

X, X_i, X_{i+1}: State vector (e.g. ozone profile)

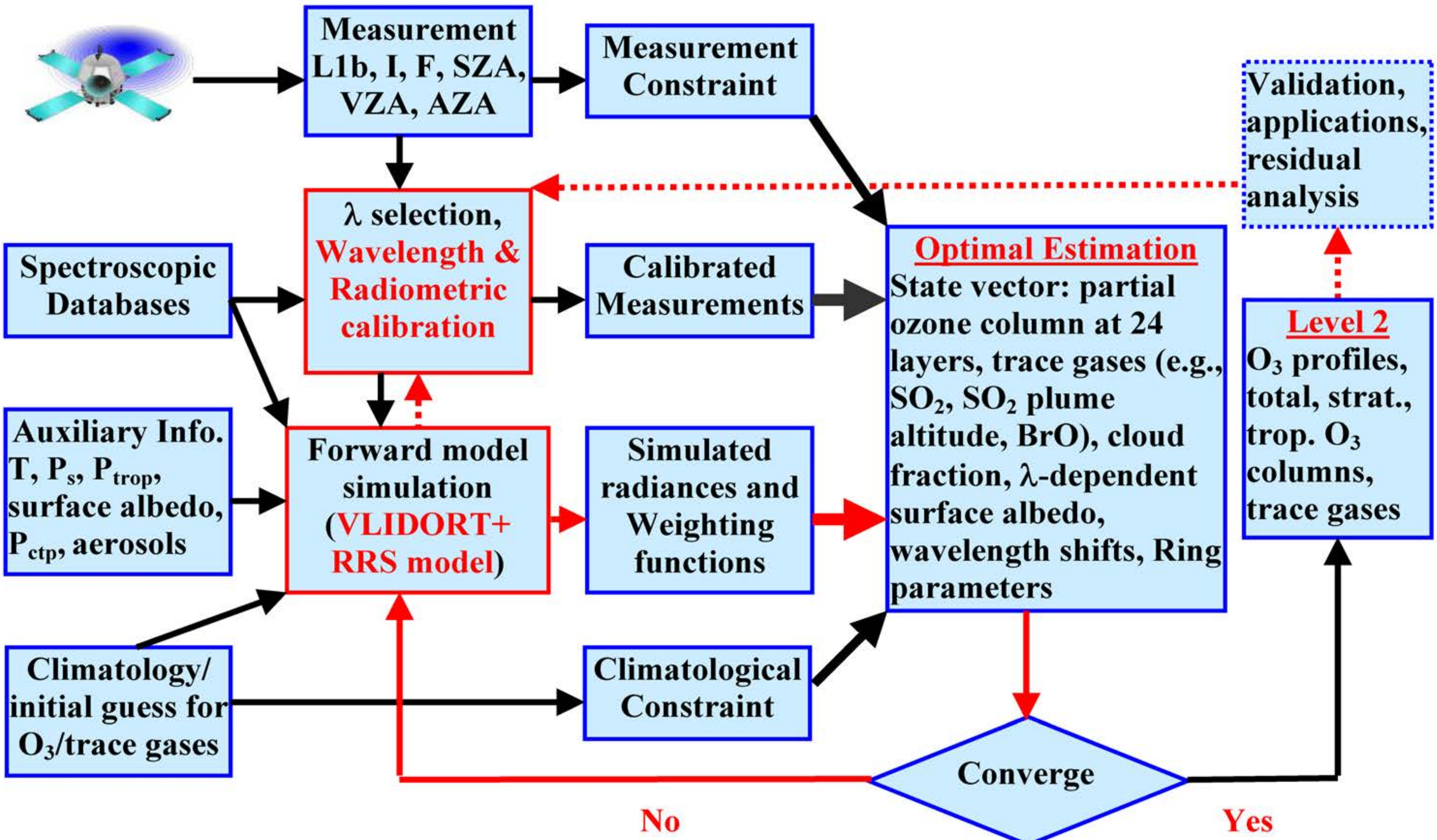
X_a: *a priori* state vector

K : Weighting function matrix, sensitivity of radiances to ozone

Sa: *A priori* covariance matrix

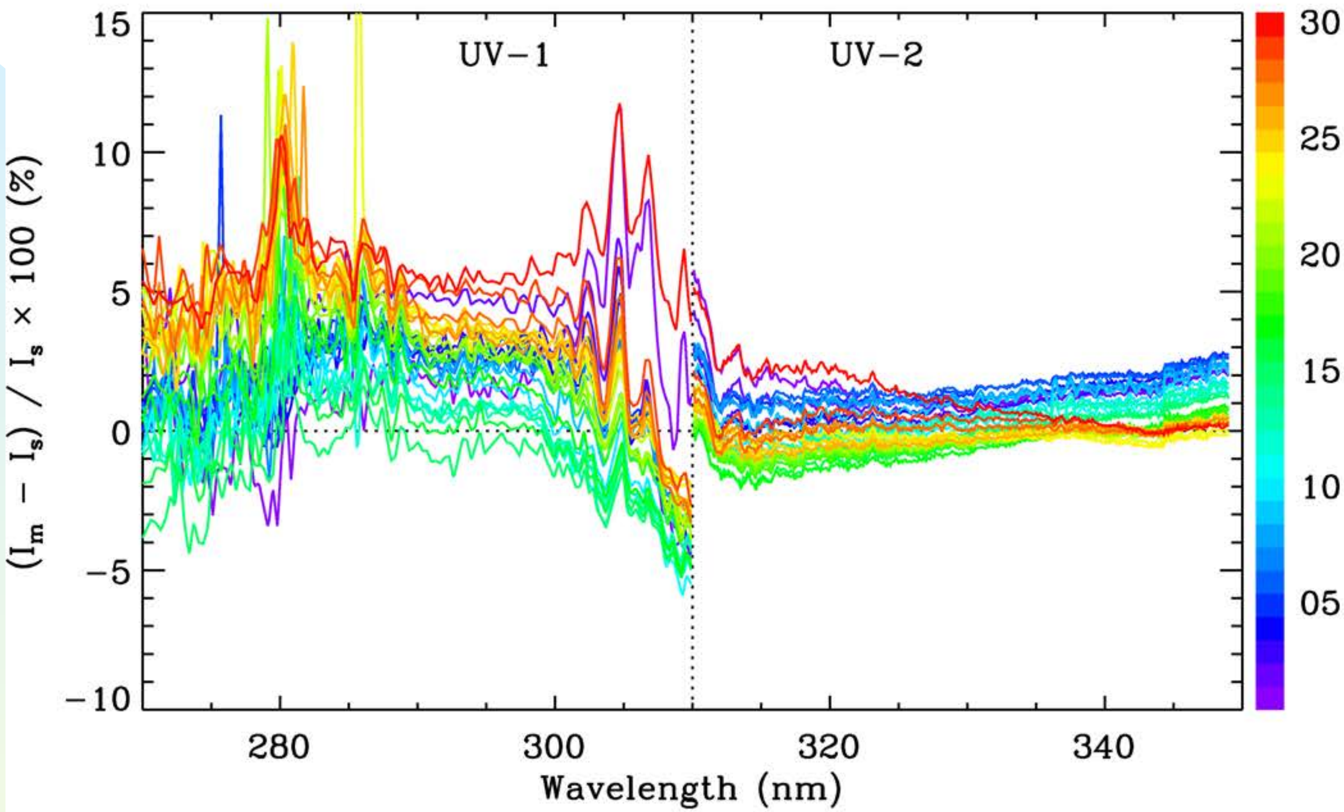
Sy: Measurement error covariance matrix

SAO OMI Ozone Profile Retrieval Algorithm



- **Keys to retrievals: accurate calibration and forward model simulations, fit the radiance spectra to ~0.1% in the 310-330 nm**

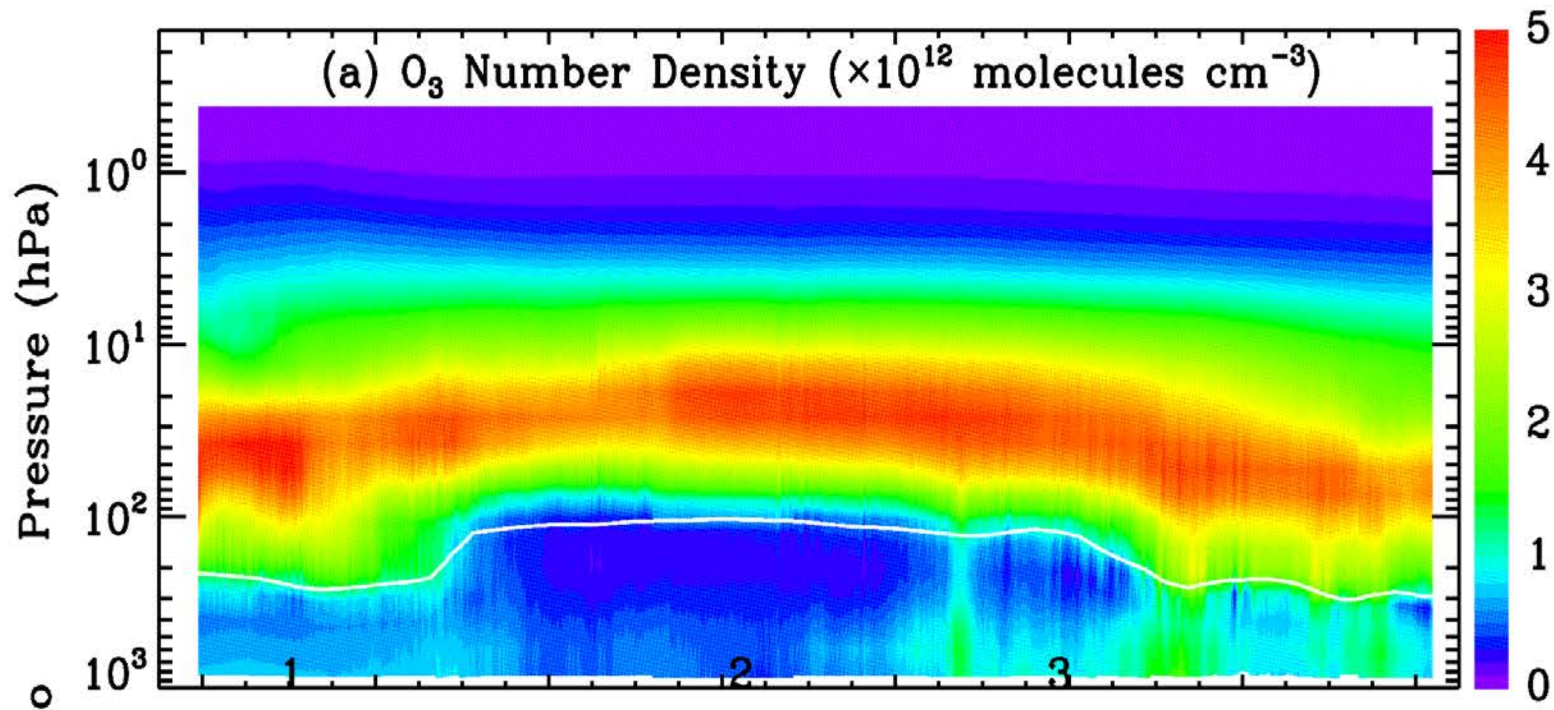
Empirical Radiometric Calibration (OMI)



- Calibrate OMI data using daily zonal mean MLS profiles and McPeters climatology in the tropics (20°S-0)
- Significant wavelength and X-track dependent biases, large discontinuity
- Correction is derived from 2 days' residuals & applied independent of time & location

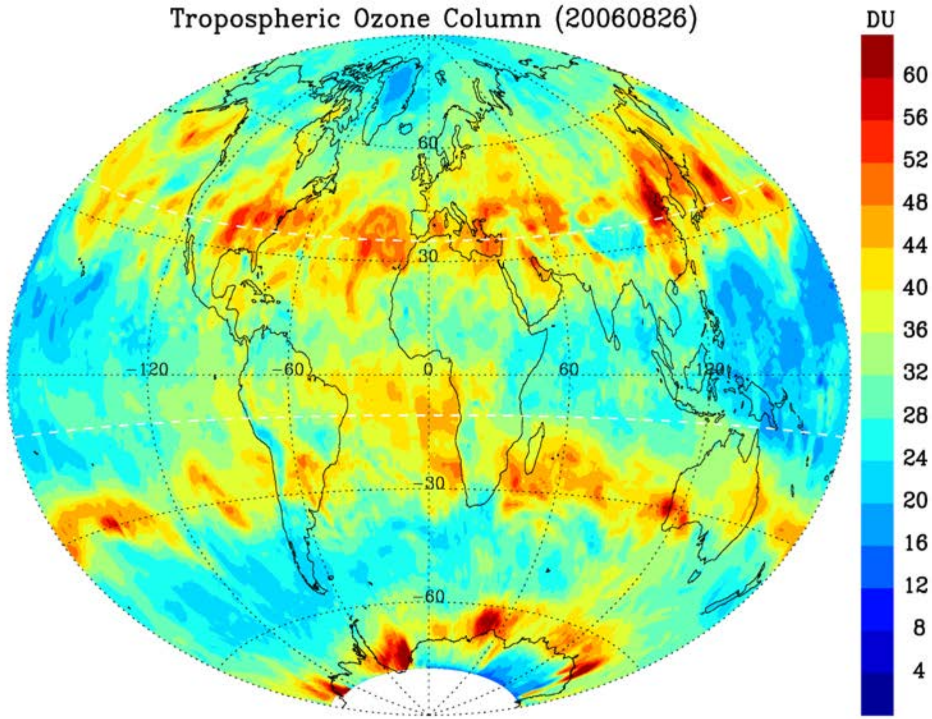
SAO OMI Ozone Profile Retrieval Algorithm

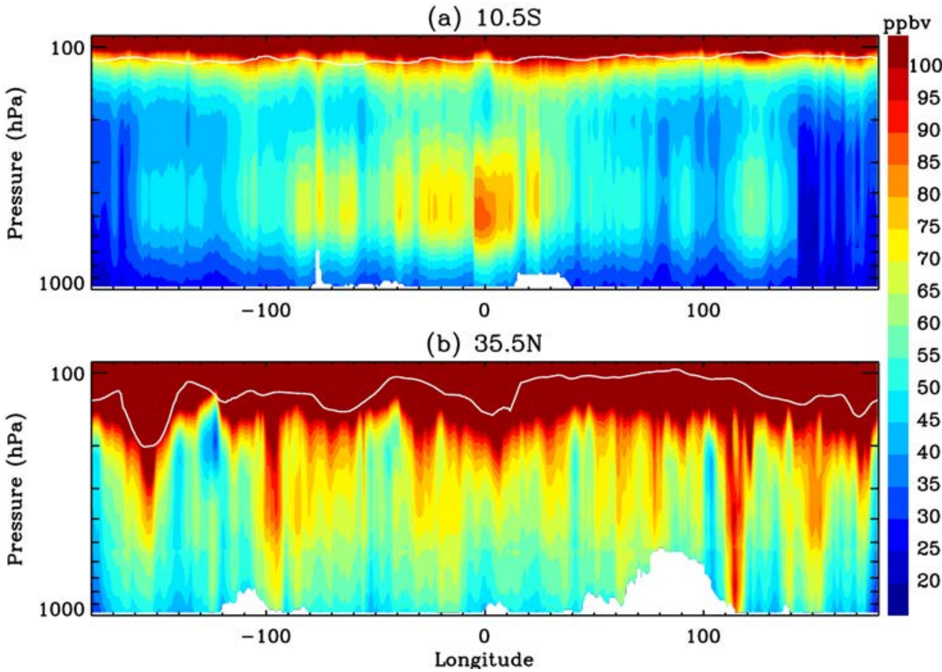
- **It is implemented in OMI SIPS : based on Liu et al. (2010) with 2 major modifications**
  - **4X binning along the track to speed up processing 52×48 km^2@nadir**
  - **A minimum floor noise of 0.4% in UV1 and 0.2% in UV2 is used to stabilize retrievals, but reduces retrieval sensitivity**
- **It produces PROFOZ: available at Aura AVDC for the entire period: http://avdc.gsfc.nasa.gov/index.php?site=1389025893&id=74**



July 11, 2006

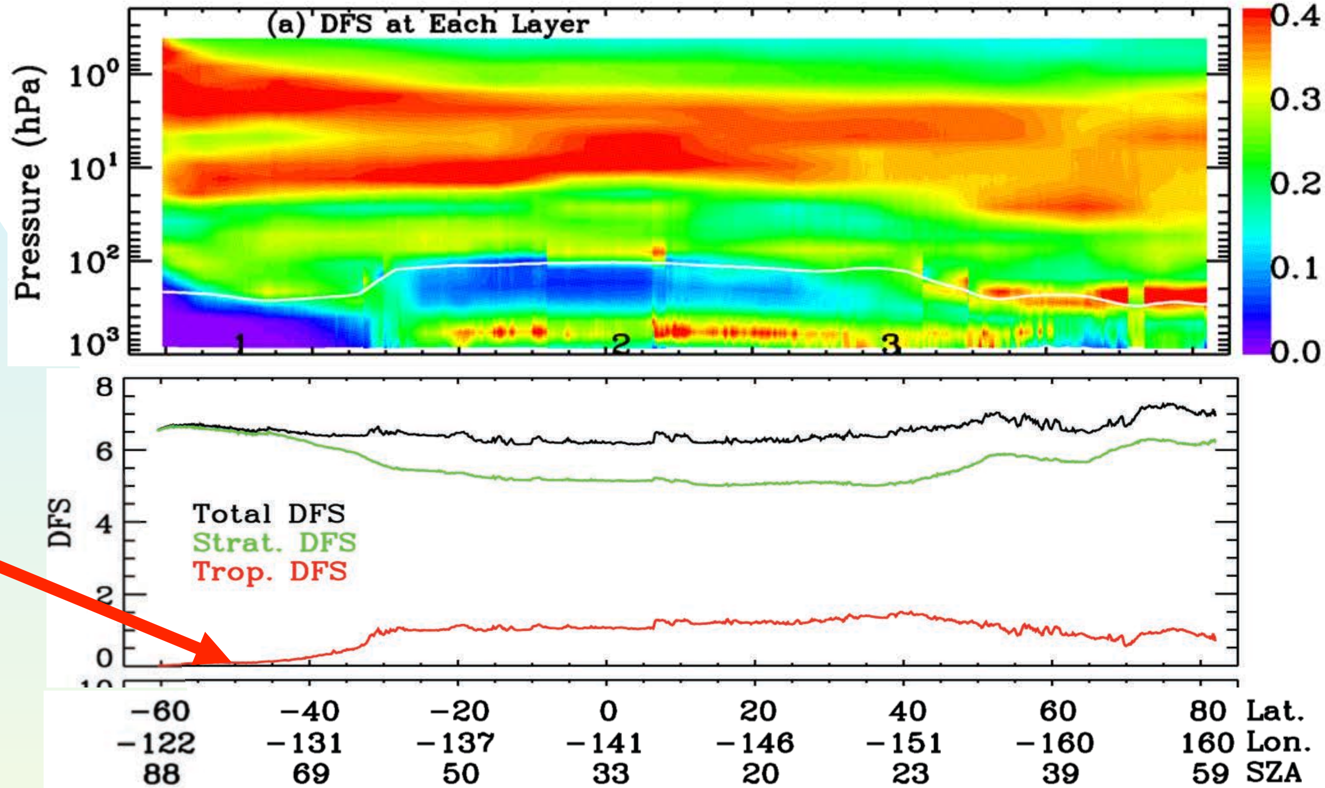
Examples of Retrievals (OMI, 2006m0826)





Retrieval Characterization: Vertical Information (OMI)

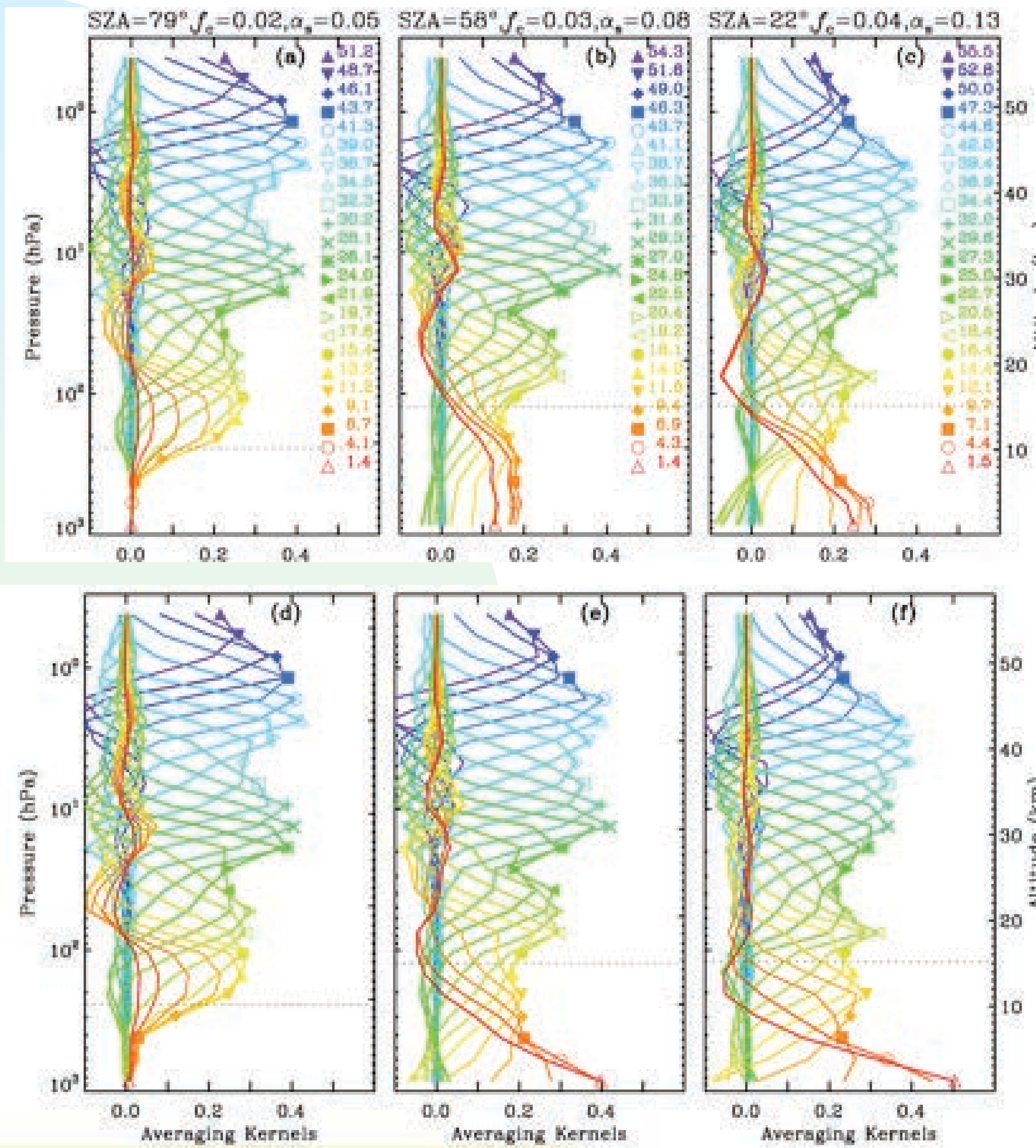
2006m0711



High SZA
(70-88)

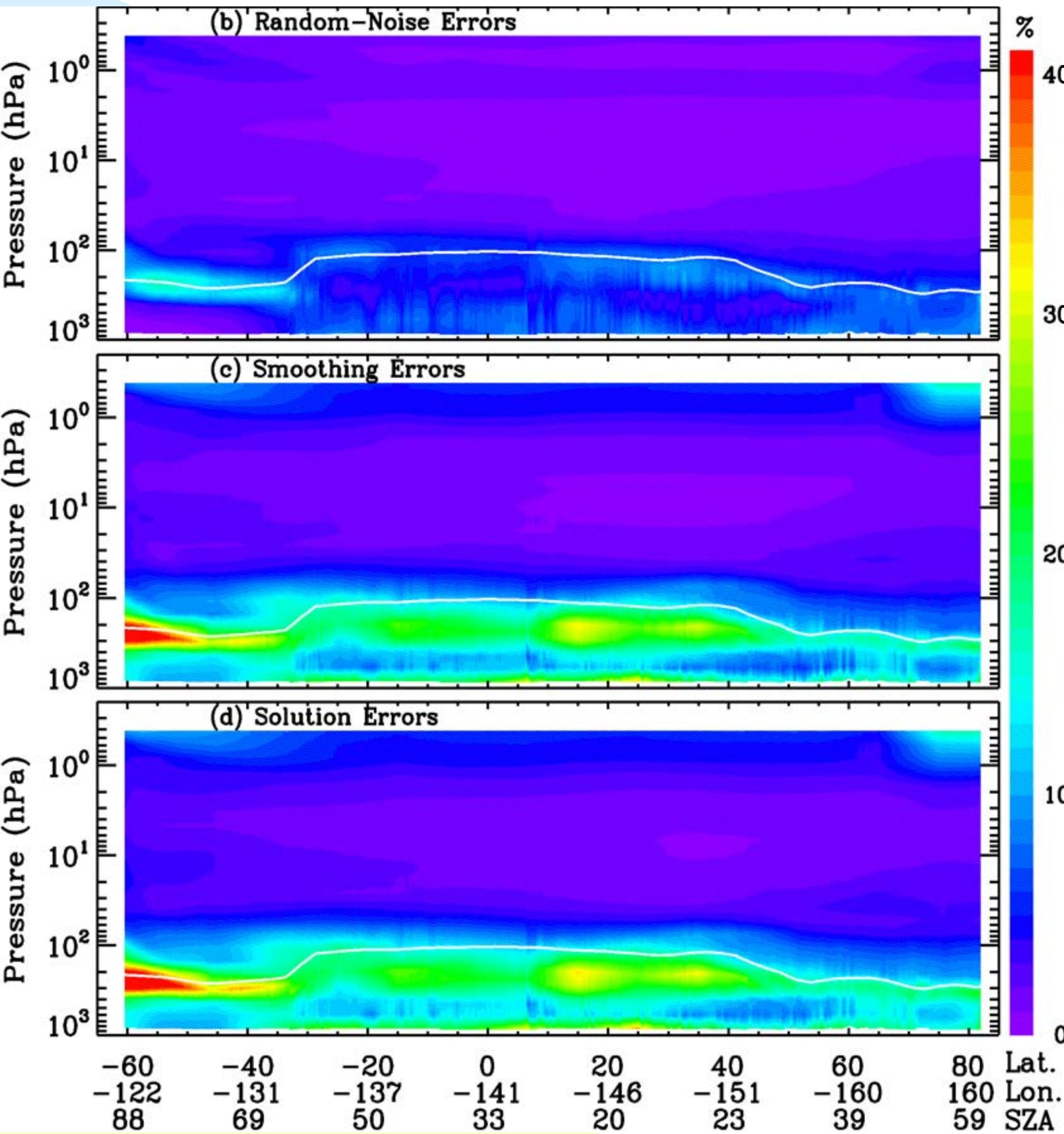
- Most of the information is in the stratosphere
- Tropical and mid-latitude summer: tropospheric O_3 information generally peaks in the 500-700 hPa layer, retrievals are effectively sensitive to ozone down to ~800 hPa.
- 6-7.3 DFS, 5-6.5 in the stratosphere, 0-1.2 in the troposphere, 2-3 below the ozone density peak

Retrieval Characterization: Vertical Information



- **Averaging kernels based on Liu et al. (2010). Retrieval sensitivity especially in the troposphere is reduced by ~0.2 in PROFOZ.**
- **Well resolved in the stratosphere with ~7-10 km FWHM, and ~10-14 km in the troposphere**
- **Significant retrieval interferences from other auxiliary parameters in the lower troposphere, and the use of 0.2% floor noise: otherwise: up to 1.8 DFS, effectively sensitive to ozone at 900-950 hPa.**

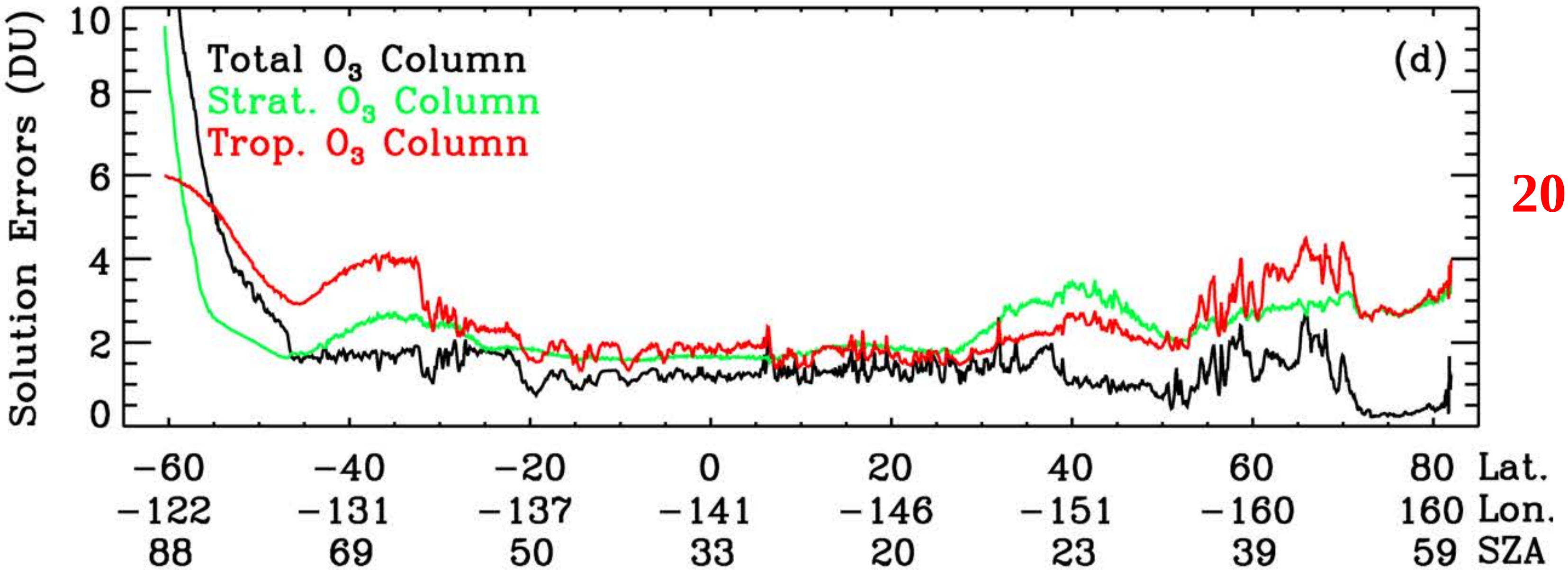
Retrieval Errors (1σ Random-Noise + Smoothing Errors)



- **Random-noise (R) errors:**
  0.6-2.5% in the middle strat., generally within 12% below
- **Smoothing (S) errors usually dominate solution errors**
- **Solution (R+S) errors:**
  1-7% in the middle strat.
  generally up to 10% in the upper stratosphere
  generally within 7-38% in the lower stratosphere and troposphere

2006m0711

Retrieval Errors (1σ Random-Noise + Smoothing Errors)

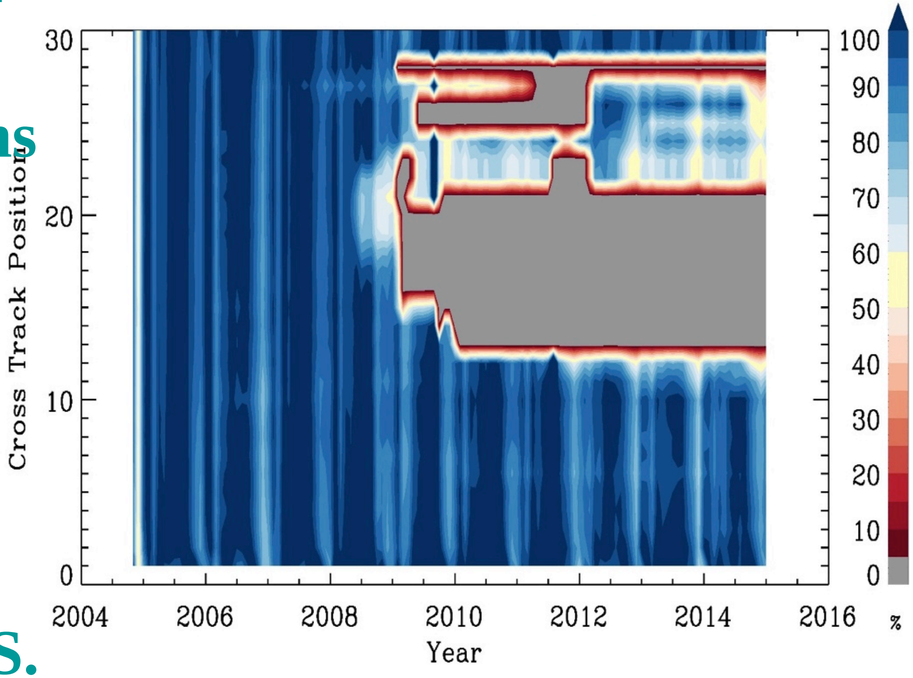


2006m0711

- **Errors (SZA < 80°):**
  - **TOZ: 0.5-3 DU, OMTO3 and OMDOAO3 errors are a few times larger**
  - **SOC: 1.5-4 DU, better than limb measurements (e.g., MLS on Aura)**
  - **TOC: 2-5 DU**
- **Validation shows that total ozone retrieval performance is better than the three operational products (Bak et al., 2015).**

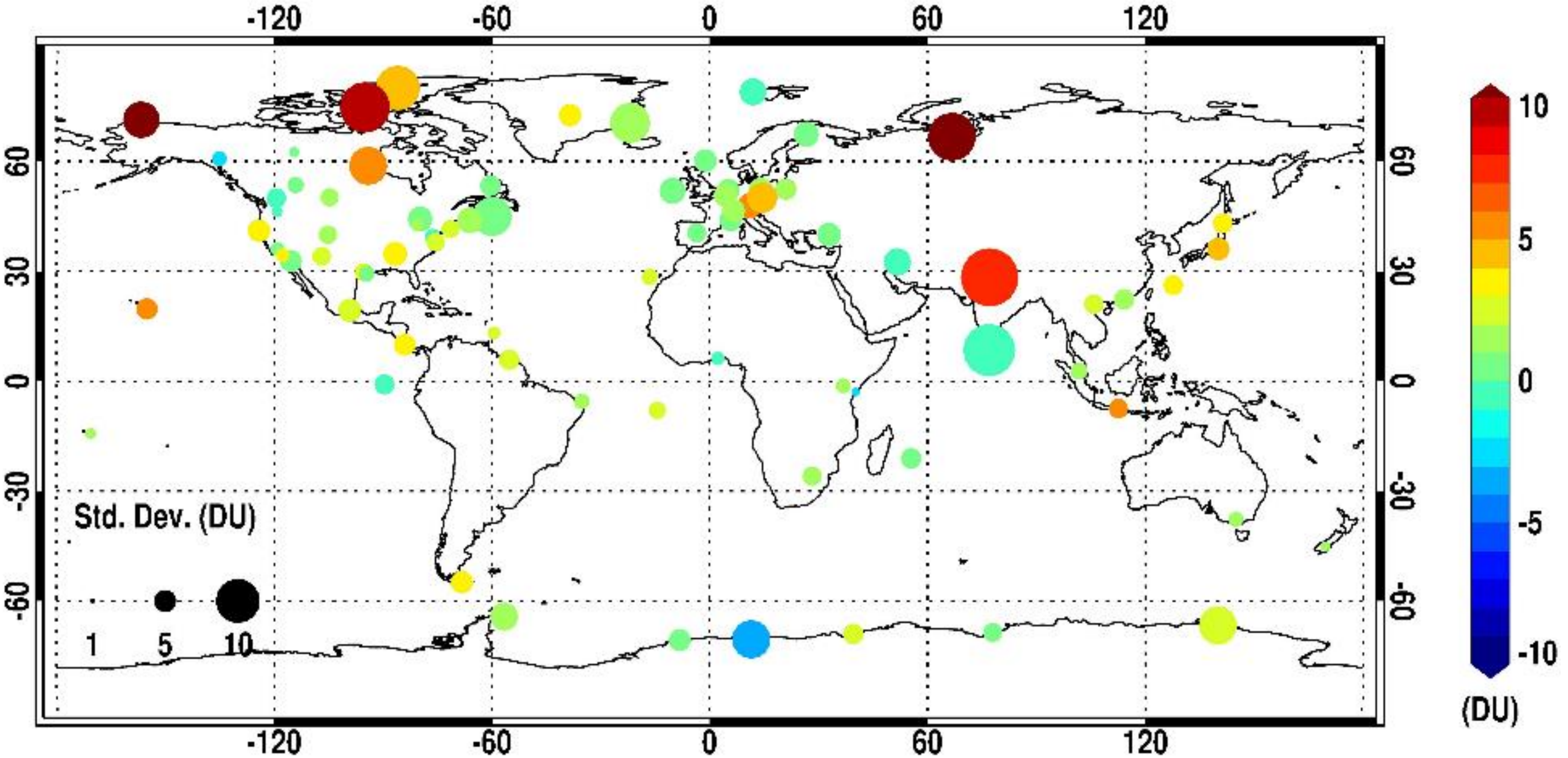
Validation of 10-year PROFOZ Using Ozonesonde and MLS

- **With 10+ years of data, what is the data quality and long-term stability? ➔Evaluate the need to perform time-dependent soft calibration for next version.**
- **OMI has Row Anomaly (RA) problem: first started in 2007 at a few positions, become serious in Jan. 2009, affecting > 1/3 positions**
- **How is the retrieval quality affected by RA? It was suggested that RA likely affects UV 1 data (therefore stratospheric ozone) at all cross-track positions.**
- **Validate using ozonesonde & MLS.**
  - ➢ **Pre RA (2004-2008)**
  - ➢ **Post RA (2009-2014)**



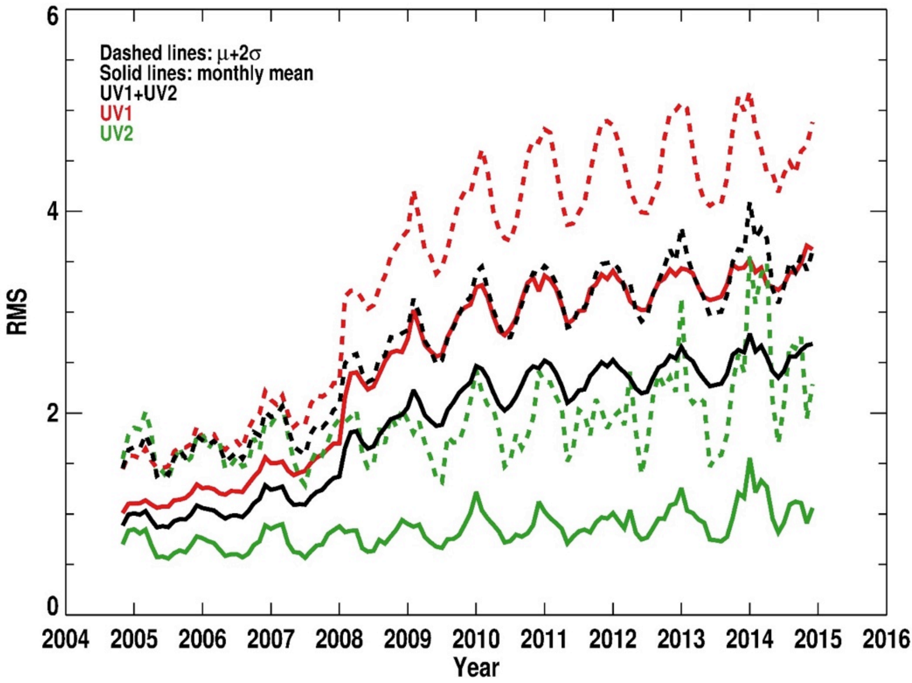
Validation with Ozonesonde

- **Ozonesonde data (~27,000 profiles) over the globe (2004-2014).**
- **~ 100 ozonesonde stations, including those from field campaigns, was obtained from Aura AVDC, WOUDC, SHADOZ, DISCOVER-AQ, etc.**
- **TOC Mean biases (MBs) mostly < 3 DU and 1σ < 6 DU except for large MBs/1σ at several N. high latitude locations, and in India due to the use of different type of sonde (India sondes)**



Validation with Ozonesonde Data

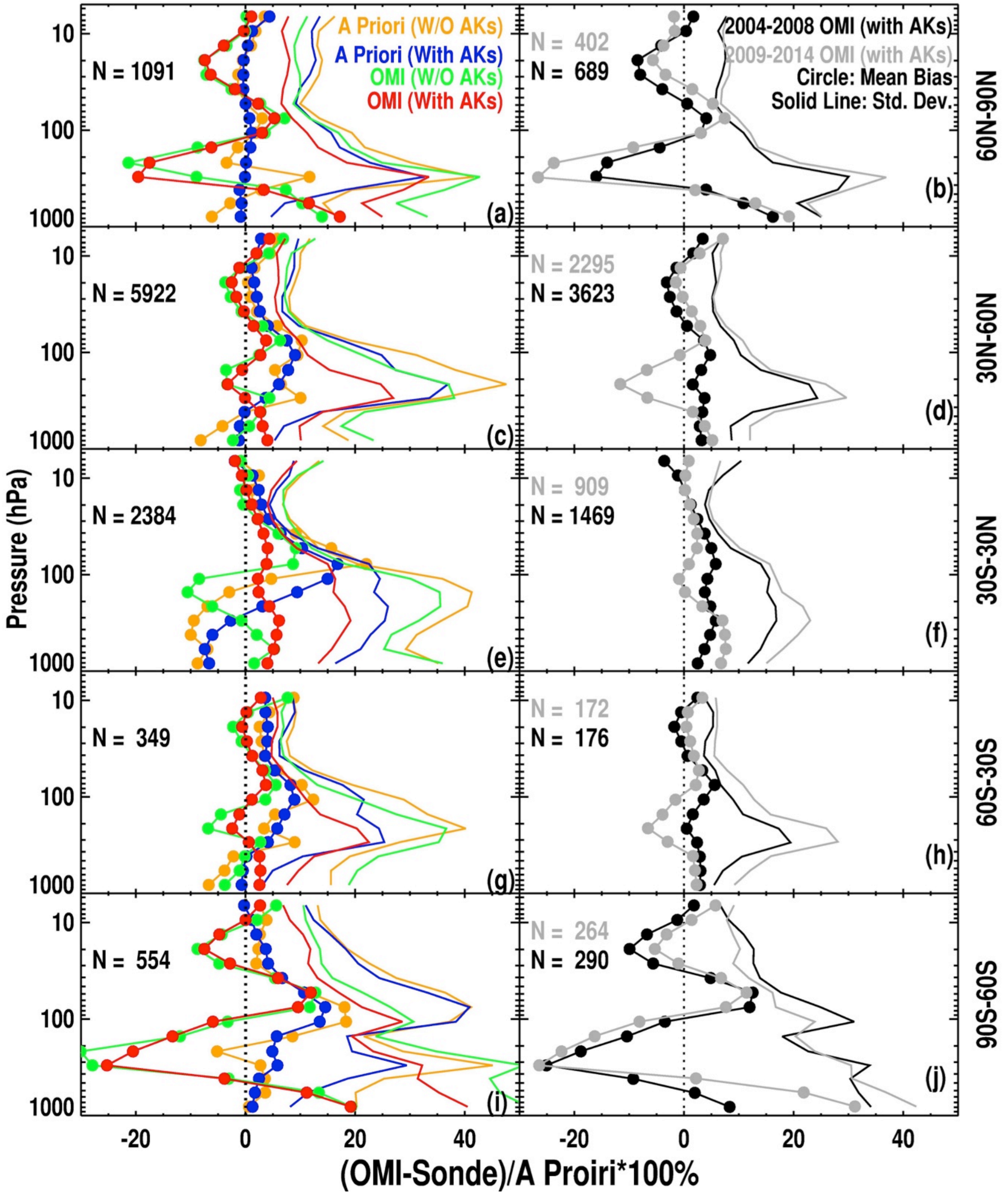
Key Thresholds	
Distance	< 100 km (nearest coincident pair)
Time	< 6 hours
R.M.S.	< mean+ 2σ
Cloud Fraction	< 0.3
Cross-Track	4-27
SZA	< 75°



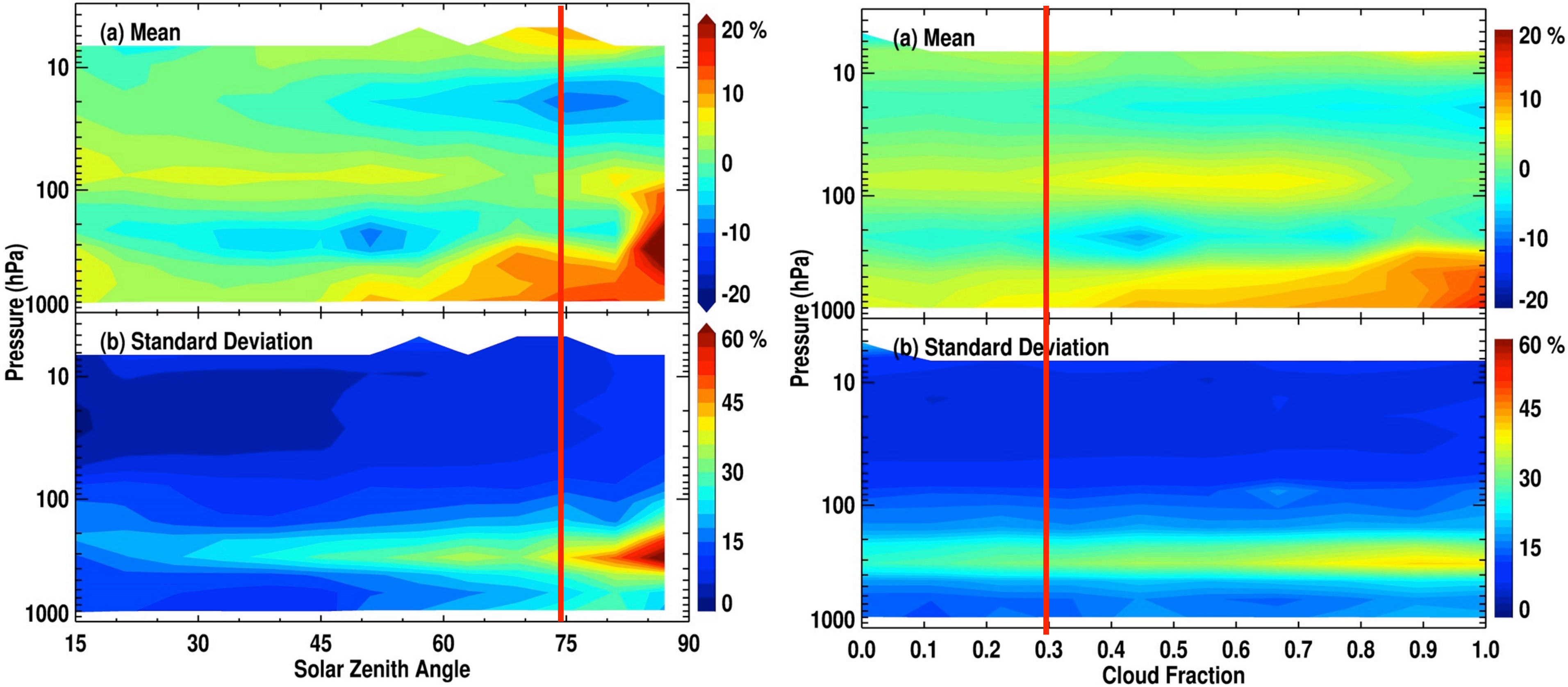
- **Fitting RMS increases with time due to increase noise and Row anomaly**

Profile Comparison

- Three periods: 2004-2014, 2004-2008 & 2009-2014.
- Better agreement in the mid-latitudes and tropics than in the high latitudes.
- Biases are within 6% in mid-latitudes and tropics, with standard deviations of up to 20-25%.
- Low mean biases (<10%) above 20 km at high latitudes.
- Pre-RA results show better comparison than post-RA with smaller standard deviations.

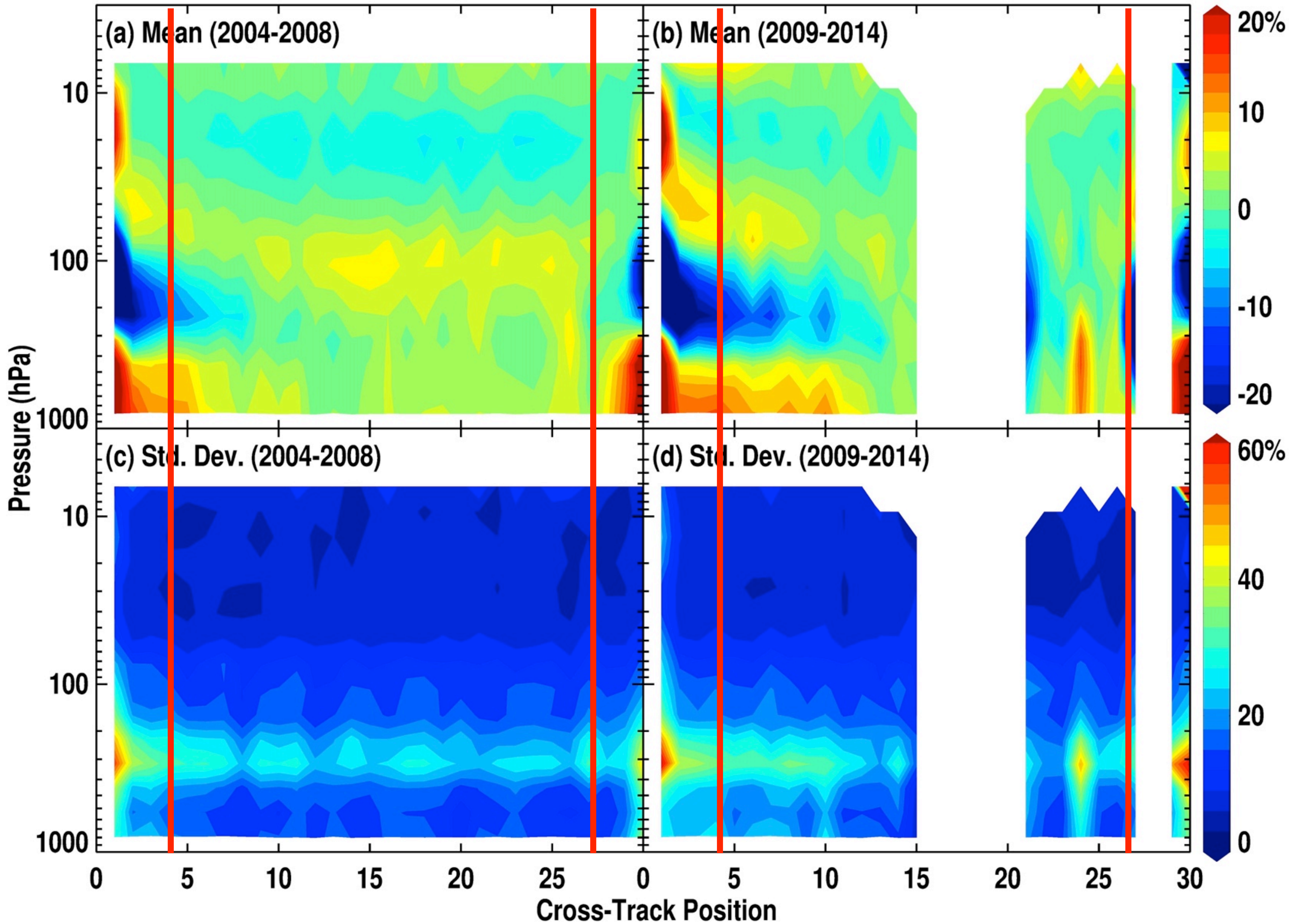


Solar Zenith Angle and Cloud Fraction Dependence



- **Poorer comparison (larger biases or altitude dependence, larger standard deviations) at larger SZAs (>75°) due to weaker signals and larger other sources of calibration errors**
- **Poorer comparison at large cloudiness (e.g., > 0.3).**

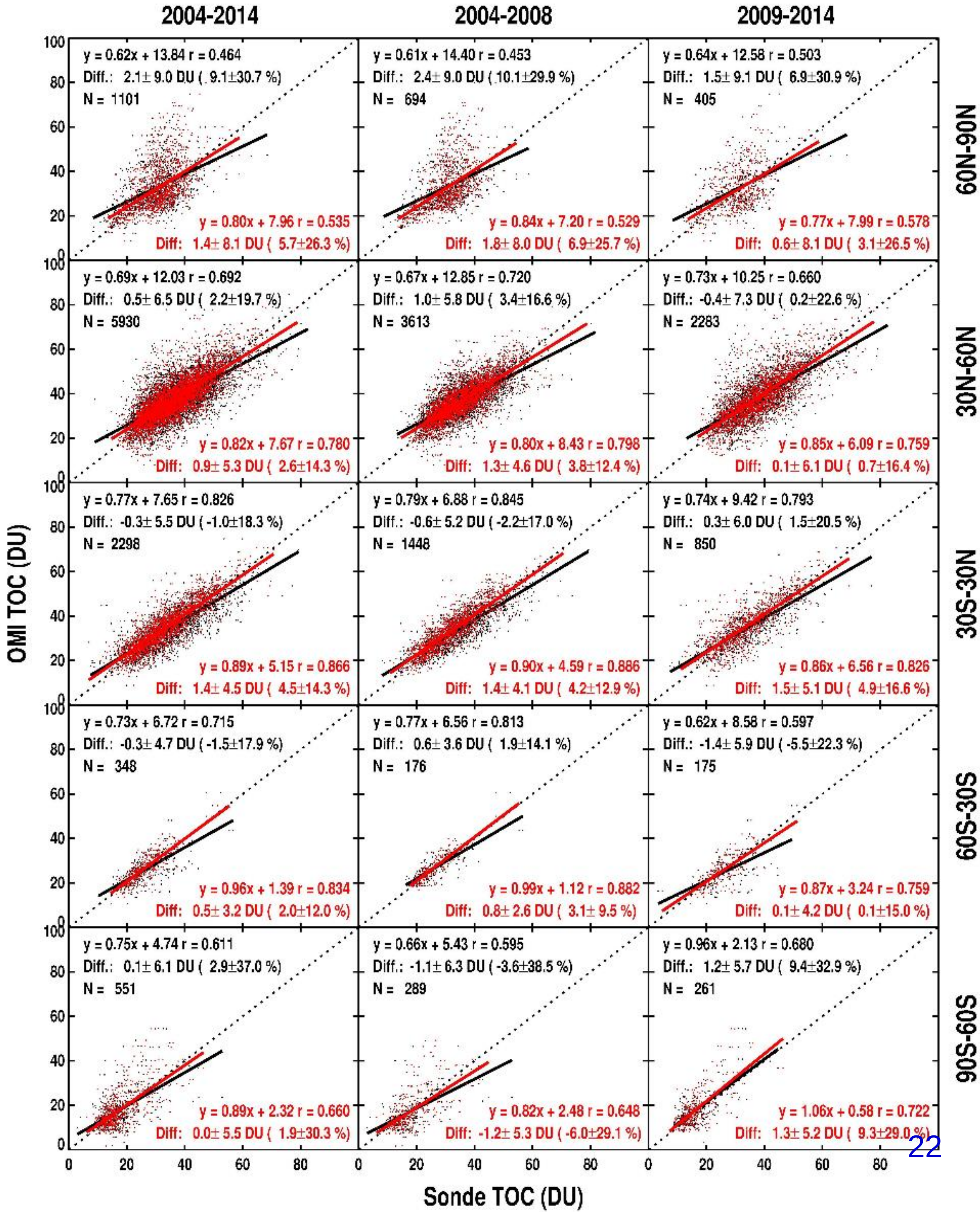
Cross-track Dependence



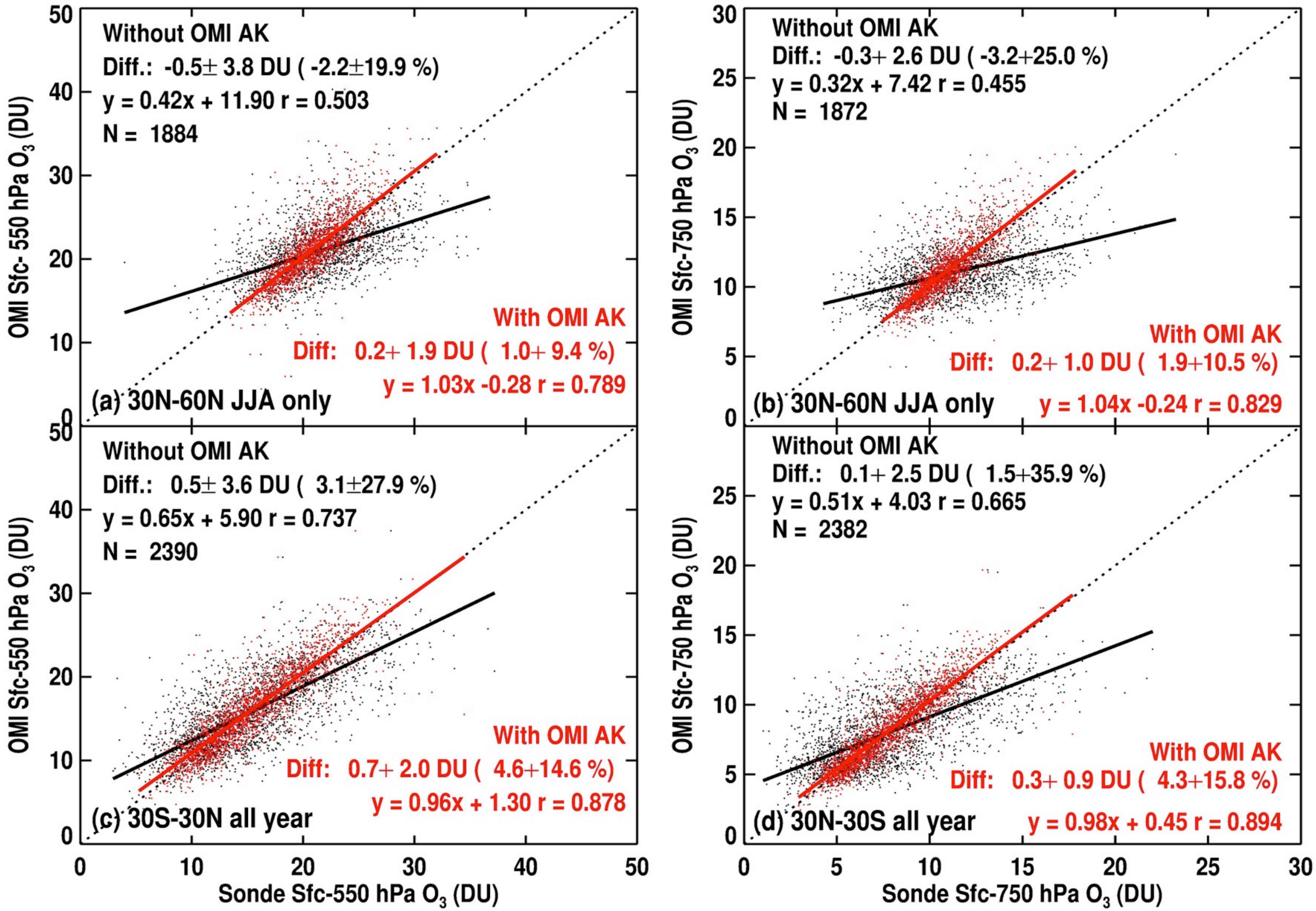
- Poorer comparison (larger biases or alt. dependence, larger std. dev.) for extreme off nadir positions (e.g., 1-4, 28-30)

Tropospheric Ozone Column Comparison

- **Surface to tropopause**
- **Much better correlation after applying OMI AKs**
- **In the tropics and middle latitudes, Mean Biases (MBs) are within 1.5 DU (6%) with standard deviations (STDs) within 15%.**
- **At high latitudes, MBs are within 2.5 DU with STDs of 30%.**
- **Smaller STDs and better correlations during the Pre-RA period (2004-2008).**



Comparison of Lower Tropospheric Ozone Columns

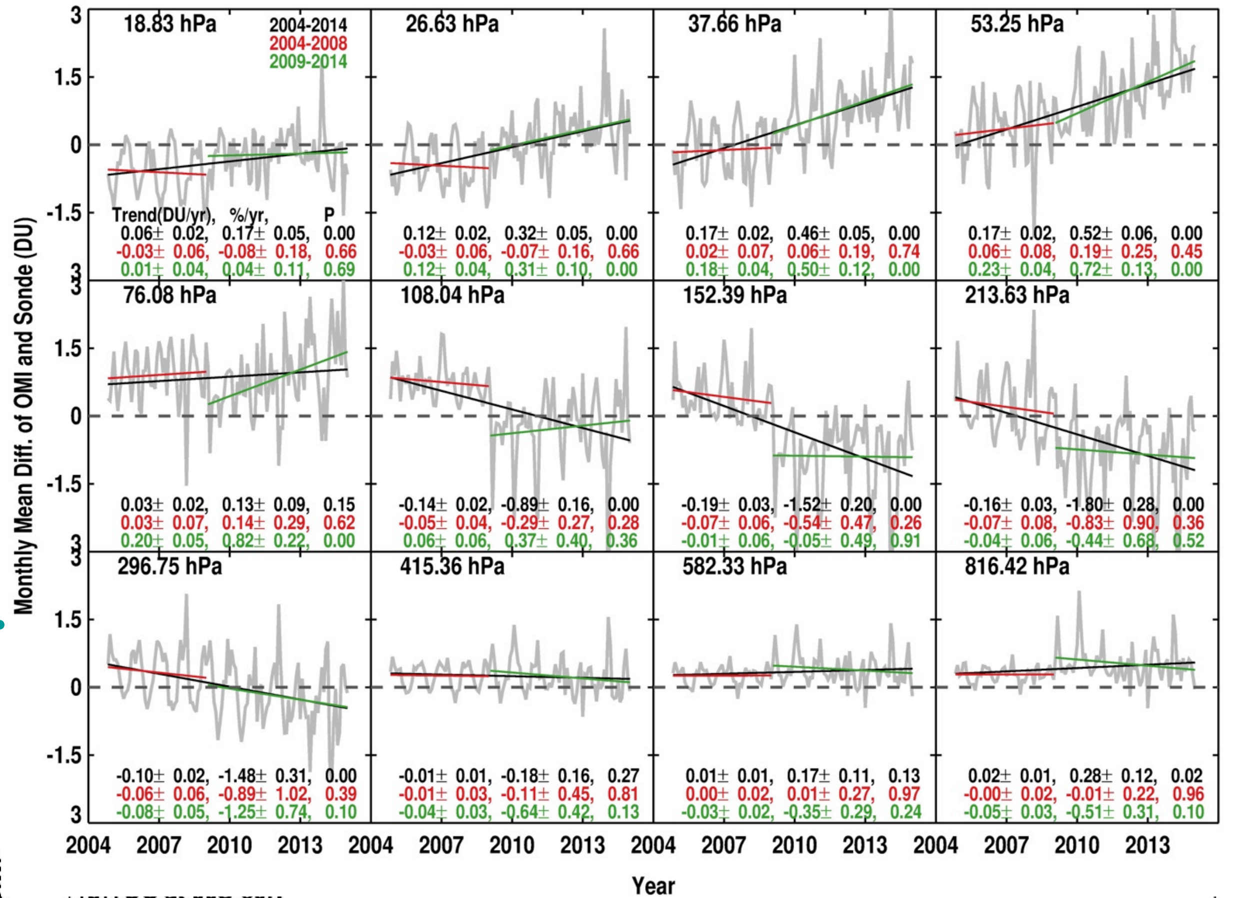


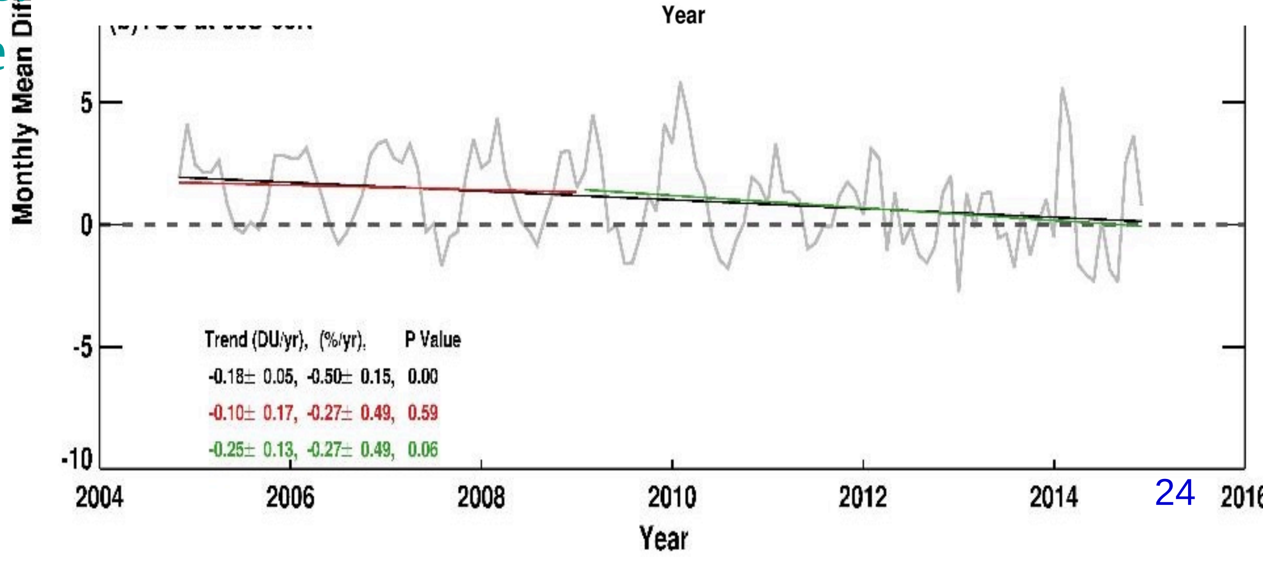
■ **Smaller slopes, correlations, larger standard deviations for layers closer to the surface due to reduced retrieval sensitivity down to the atmosphere**

Bias Trends

- Significant trends in mean biases vs. ozonesonde at individual layers or in Tropospheric Ozone Column especially during the post-RA period.

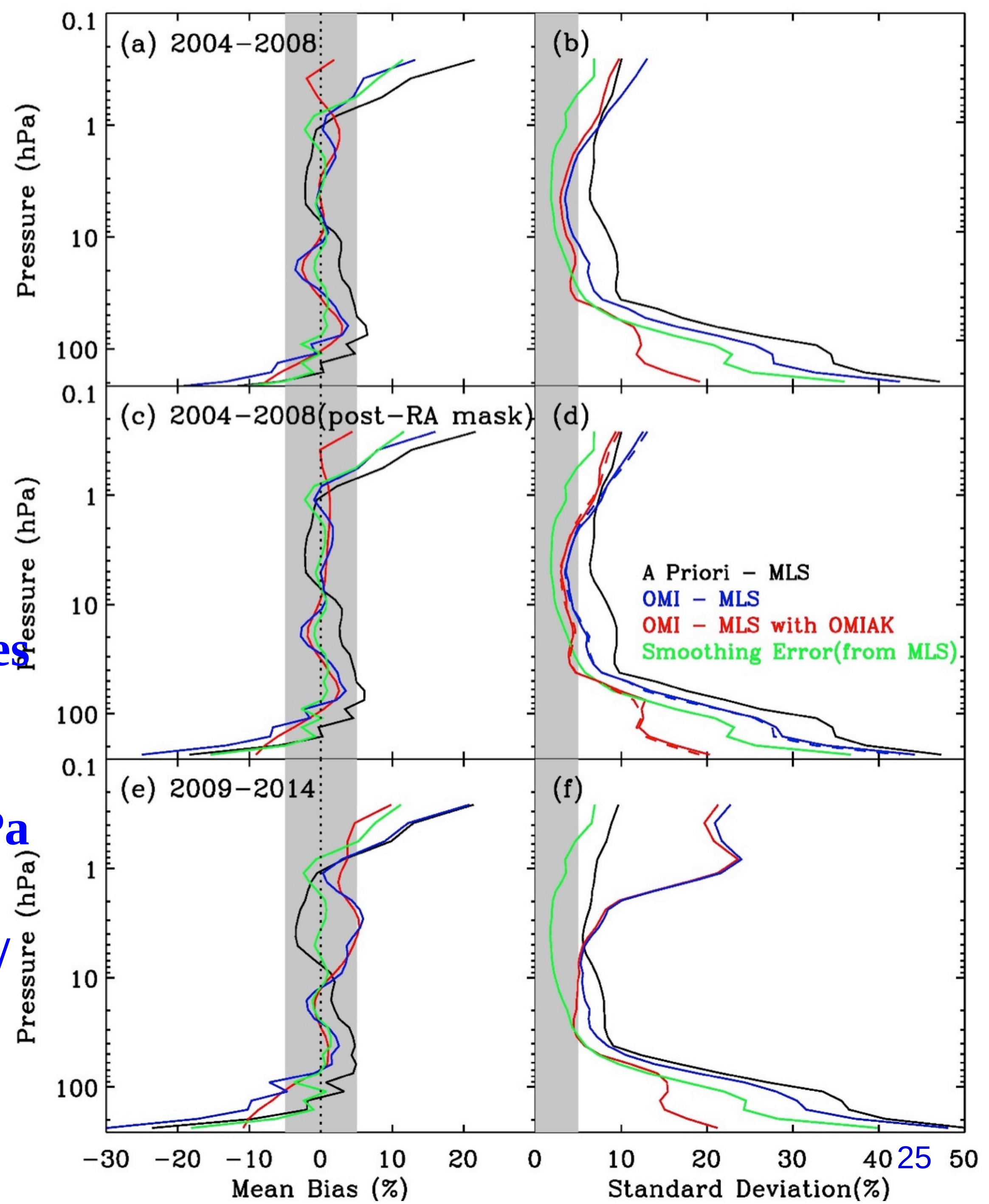
- Need to improve OMI's radiometric calibration vs. time especially during the post-RA period to maintain the long-term stability of the product.



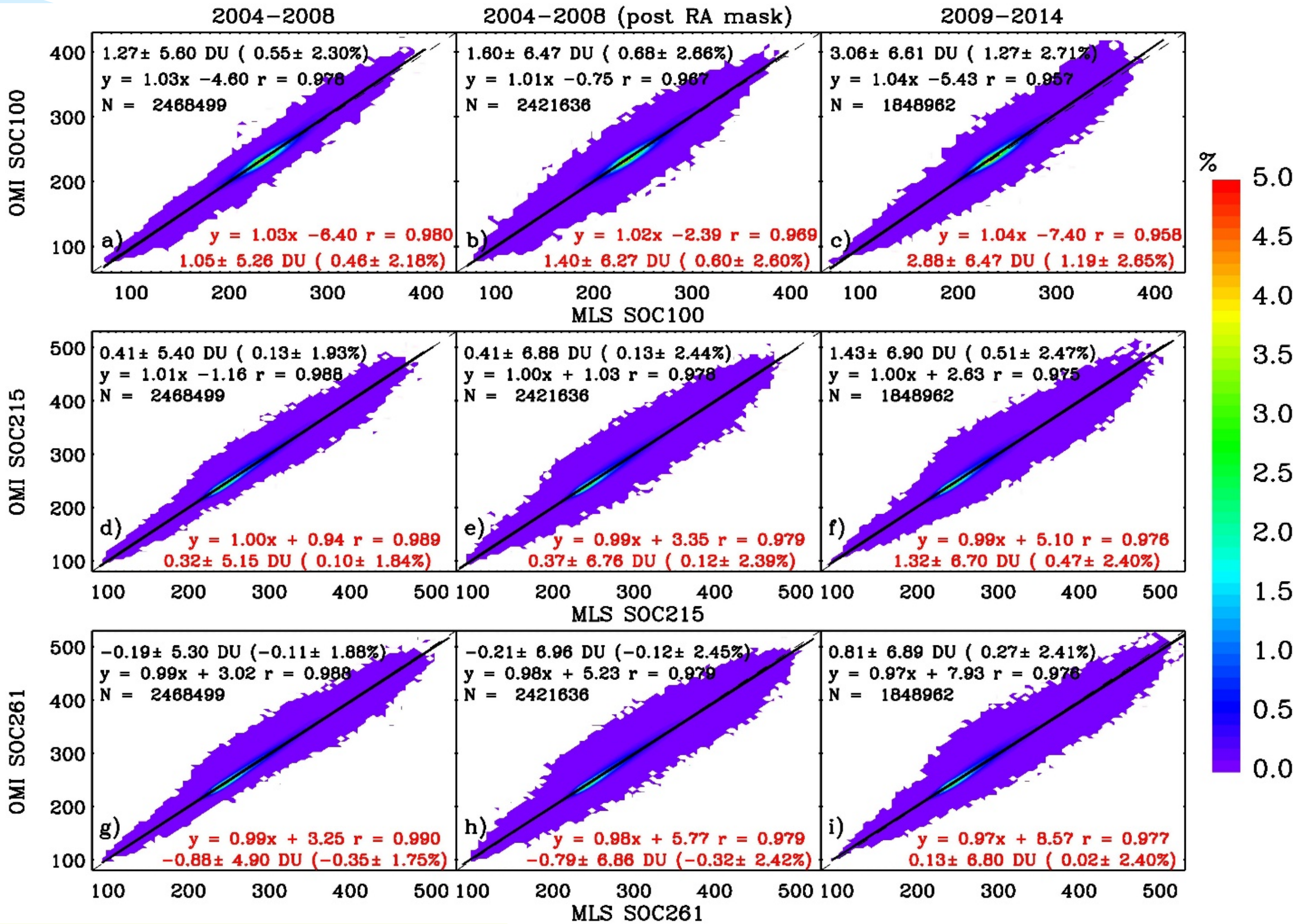


Validation with MLS

- MLS V4 O_3
- During post-RA period, no OMI/MLS collocation, use nearest MLS data.
- For pre-RA period, comparisons with either collocated MLS or post-RA masked MLS are similar.
- Pre-RA: **Global mean biases generally within 5%, with 1σ of 3-5% at 2-30 hpa, increasing to 10% above 1 hPa and to 20% at 261 hPa.**
- Post-RA: **slightly larger 1σ/ biases below 3 hPa, much larger 1σ at higher altitudes, suggesting UV1 is affected by RA for non-flagged pixels.**



Validation with MLS



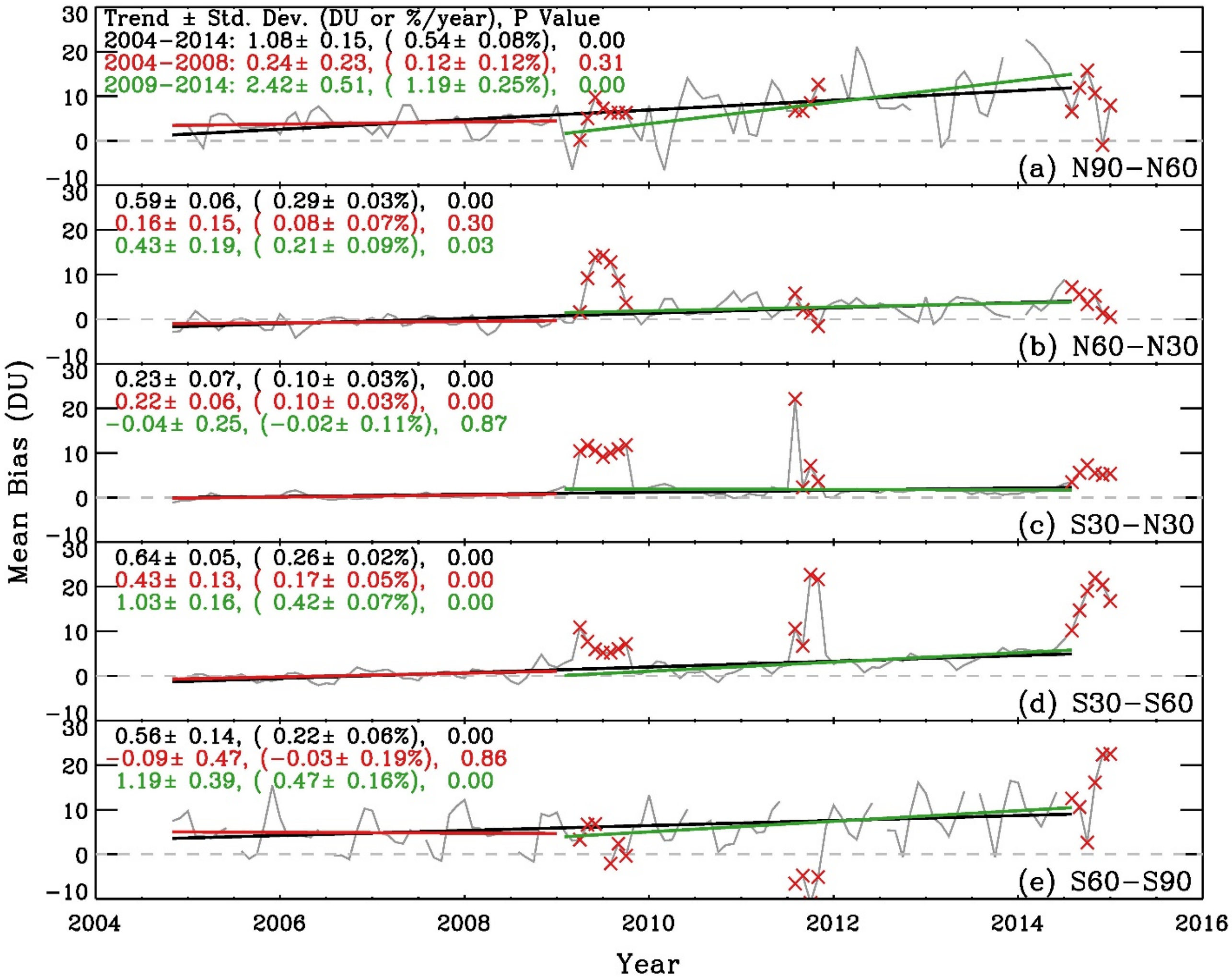
SOC down to 100 hPa

SOC down to 215 hPa

SOC down to 261 hPa

- **Excellent agreement with MBs typically within 2 DU (0.7%) and 1σ of ~1.9-2.3% for collocated OMI/MLS, 1σ 0.3-0.6% larger for 2004-2008 with post-RA mask or 2009-2014.**

Bias Trend in SOC down to 100 hPa



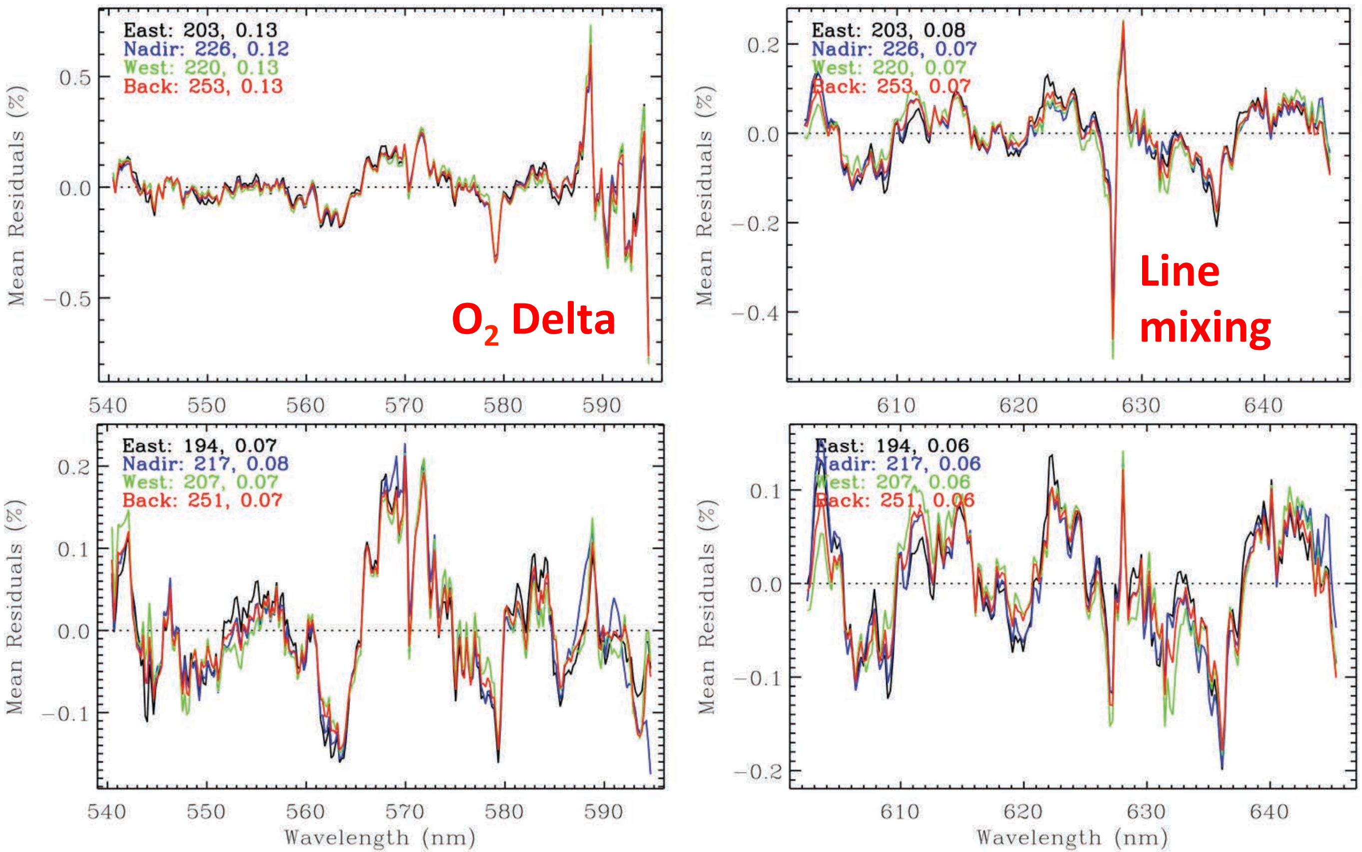
■ **Post-RA: a few periods with very large biases, larger variation, significant trend**

Adaption of OMI Algorithm for TEMPO

- **Adapted from GOME (Liu et al., 2005), OMI (Liu et al., 2010), GOME-2 (Cai et al., 2012): Spectral fitting + VLIDORT + OE**
- **Fitting windows: 290-345 nm (UV), 540-650 nm (Visible)**
- **O_3 profile at > 24 layers (add several 1 km layers near the surface) from surface to ~60 km, derive 0-2 km ozone column in addition to total, stratospheric, and tropospheric ozone columns**
- **Tropopause-based O_3 profile climatology (Bak et al., 2013): further improvement to account for diurnal variation**
- **Meteorological data (temperature profiles, surface pressure, and tropopause pressure): North American Mesoscale (NAM) Forecast System grid 227 with 5-km resolution**
- **Speedup radiative transfer calculation: look-up table correction and/or fast Principal Component Analysis (PCA) LIDORT**

Adaption of OMI Algorithm for TEMPO

- Important to account for the temperature-dependence of the O_2-O_2 cross sections using cross sections by Thalman et al. (2013).
- Line-by-line calculations of O_2 and H_2O cross sections from HITRAN 2012 accounting for T- and P-dependence with solar I_0 correction, with additional O_2 delta band, empirical correction (O_2 line mixing)

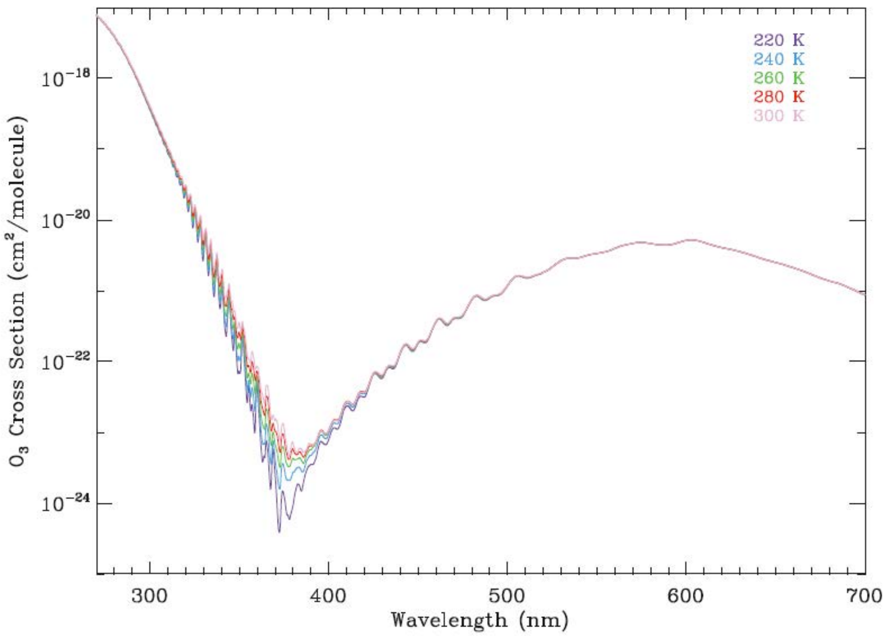


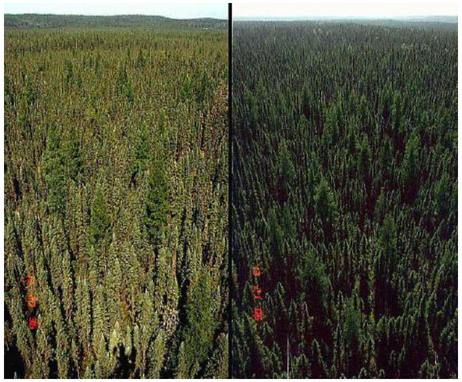
Residuals before new delta band and empirical correction

Residuals after new delta band and empirical correction (note smaller y-axis range)

Motivations of Developing Climatology of Surface Albedo Spectra

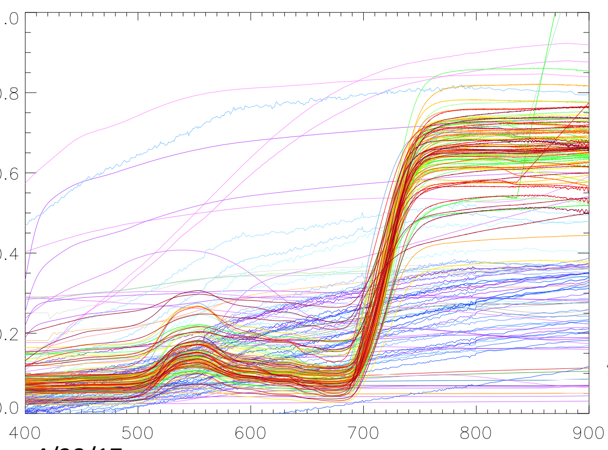
- **Ozone has weak spectral features in the Chappuis band**
- **But retrieval is very sensitive to errors in surface reflectance**
  - Spectral variation
  - Dependence on land cover
  - Changes with viewing geometry

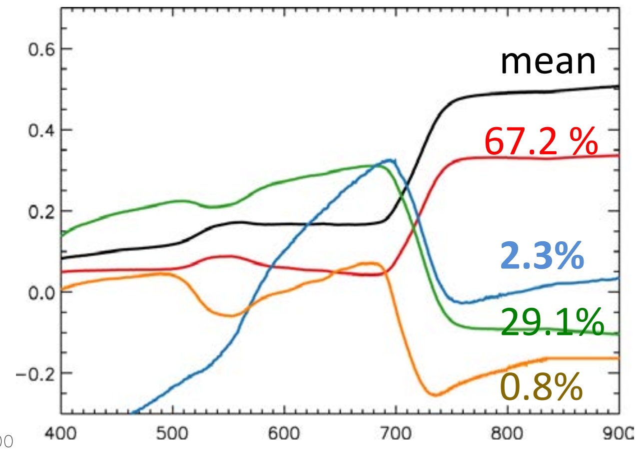




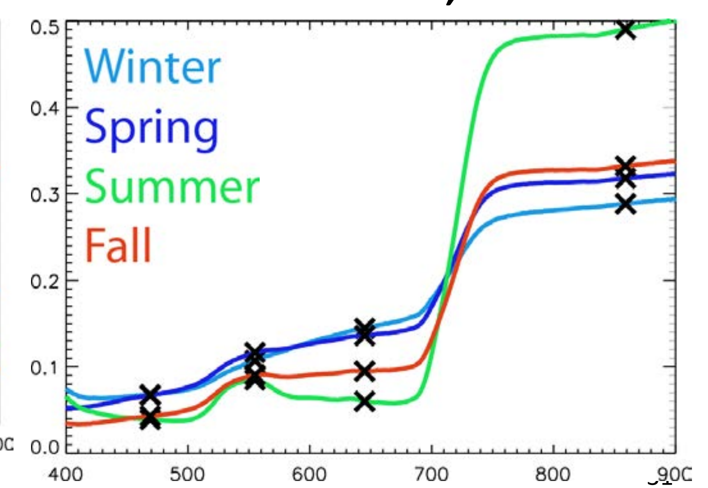
Development of A Climatology of Visible Surface Albedo Spectra

- **Developed visible surface albedo spectrum (Zoogman et al., 2016)**
  - **Lab spectra (400-900 nm) of possible ground cover including vegetation, soils, rocks, manmade, water, snow, from ASTER, USGS, MPI/Wagner's group**
  - **Empirical Orthogonal Function (EOF) analysis of shows that first 4 EOFs can explain more than 99.5% of the variance over land**
  - **Mean snow/ice (ASTER) and water over ocean spectra (USGS)**
  - **Combine EOFs+snow/ice+water with 10-year (2002-2011) average high resolution (30 arc s) MODIS BRDF climatology (466, 555, 645, 859 nm over land only) or GOME-2 surface albedo climatology (15 wavelengths in 400-900 nm, both water & land)**





Forested Scene, NY State



Surface Albedo Treatment and Fitting

- **Assumption of Lambertian surface**
- **UV: initialize albedo from climatology at 342 nm, and fit constant albedo in band 1a and albedo polynomials in band 2b (e.g., 2nd)**
- **Visible over land: Combine land EOFs and MODIS (blue sky albedo) to initialize visible surface reflectance spectrum and further fit surface spectra using 2 approaches as follows**

MODIS BRDF kernel parameters (land) at GOME-2 footprint

Viewing geometry

Directional, black sky, white, blue sky albedo

4 EOFs with MODIS Spectral Response

Initialize surface albedo spectrum $a_{\lambda 0}$

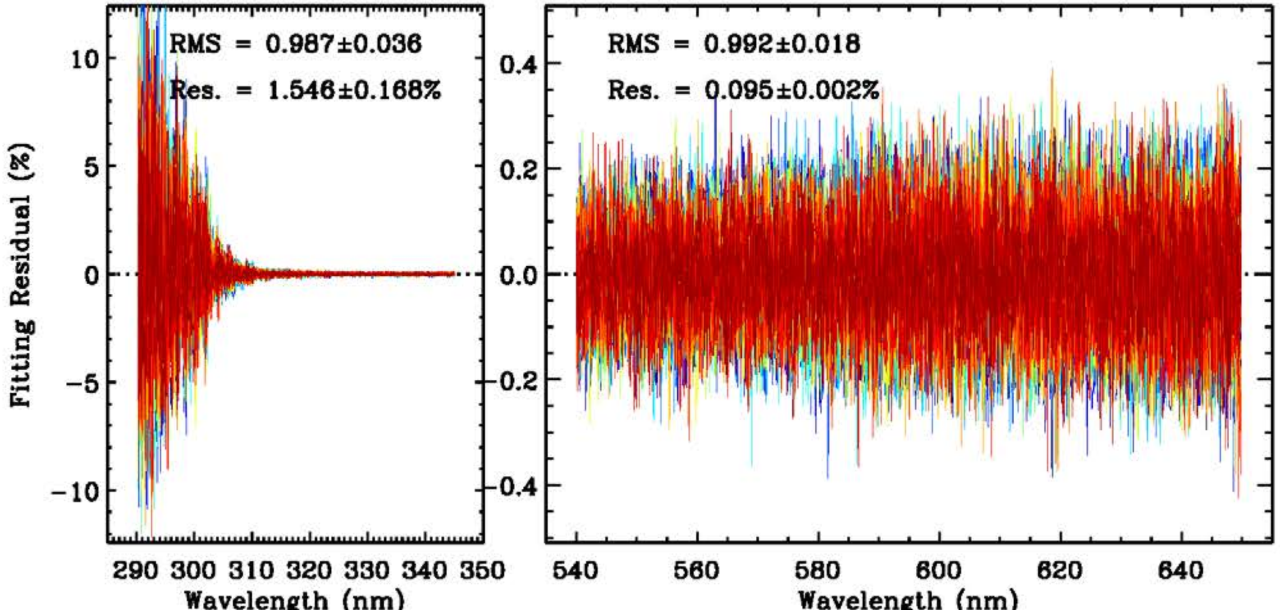
1. Albedo scaling: $a_\lambda = a_{\lambda 0} \sum_{i=0}^{n} c_i (\lambda - \lambda_{avg})^i$

2. Fit EOFs: $a_\lambda = a_{\lambda 0} + \sum_{i=0}^{n} c_i \mathrm{EOF}_i$

- **Visible over snow/ice or water surface: scale average snow/ice spectrum or water albedo spectrum**
- **Key: use fewer surface albedo parameters that increase O_3 retrieval sensitivity while adequately fit radiance spectra**

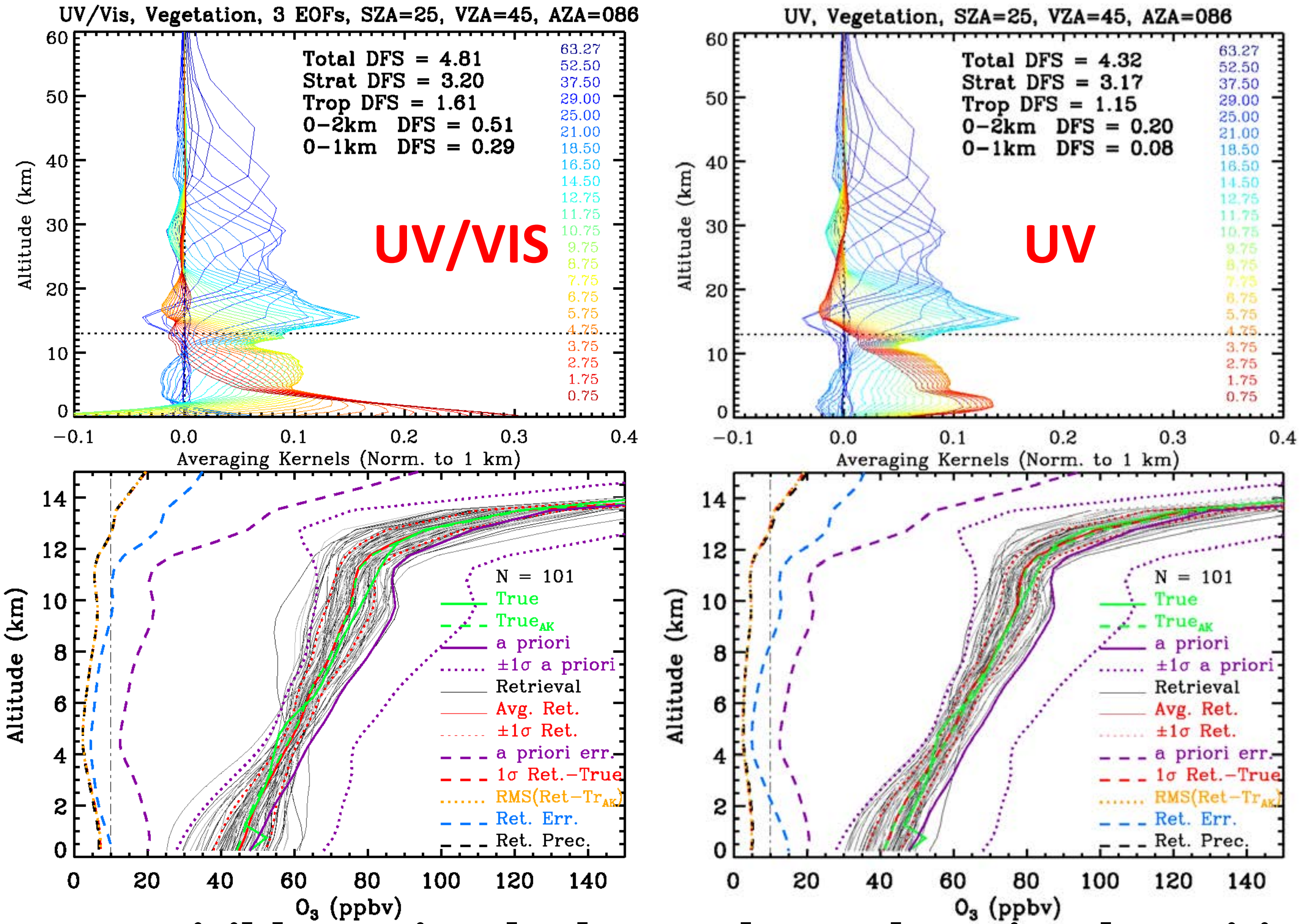
Perform Synthetic Retrievals to verify UV/Visible O_3 Profile Algorithm

- **Verify the algorithm:** iterative nonlinear retrievals (simultaneous fitting of surface parameters) from simulated radiances to show that retrievals are self-consistent with true profiles to within retrieval uncertainty
- **Tested nonlinear retrievals under clear-sky conditions**
  - 3 vegetation, 3 soil/desert, snow/ice, water with diff. TEMPO viewings, O_3 amounts for both UV only (290-345 nm) and UV + visible (290-345, 540-650 nm) retrievals
  - Each test consists of the same simulated radiance added with 101 different sets of TEMPO random noise



- **Fitting RMS (ratio of fitting residuals to measurement precisions) is almost 1 for both UV, and visible regions.**

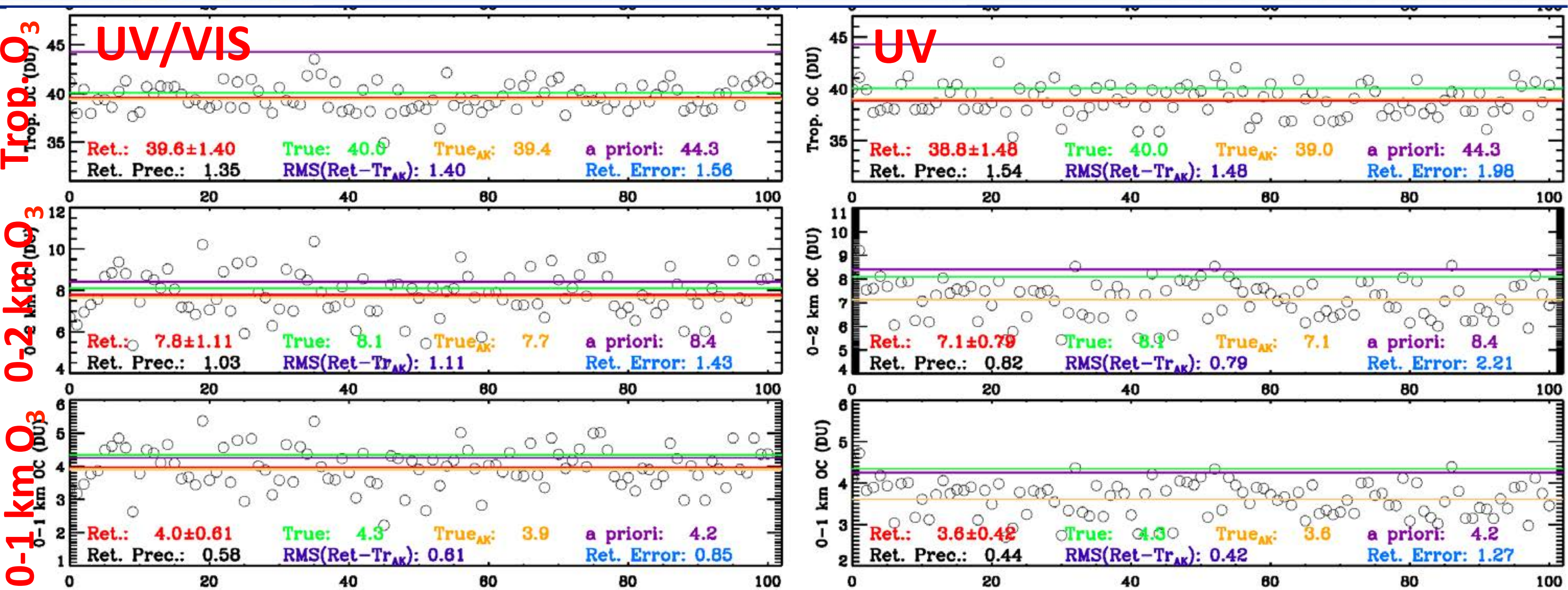
Example of Synthetic Nonlinear Retrievals: Vegetation, UV/VIS vs. UV



- Fitting 1st-order albedo polynomial in UV and 3 EOFs in the visible.
- Both UV only and UV/visible retrievals are verified for all the cases.

- UV/visible retrievals show enhanced retrieval sensitivity to lower tropospheric ozone, better agreement, smaller retrieval errors (~15% vs. ~10%) but larger retrieval precision in the bottom layers.

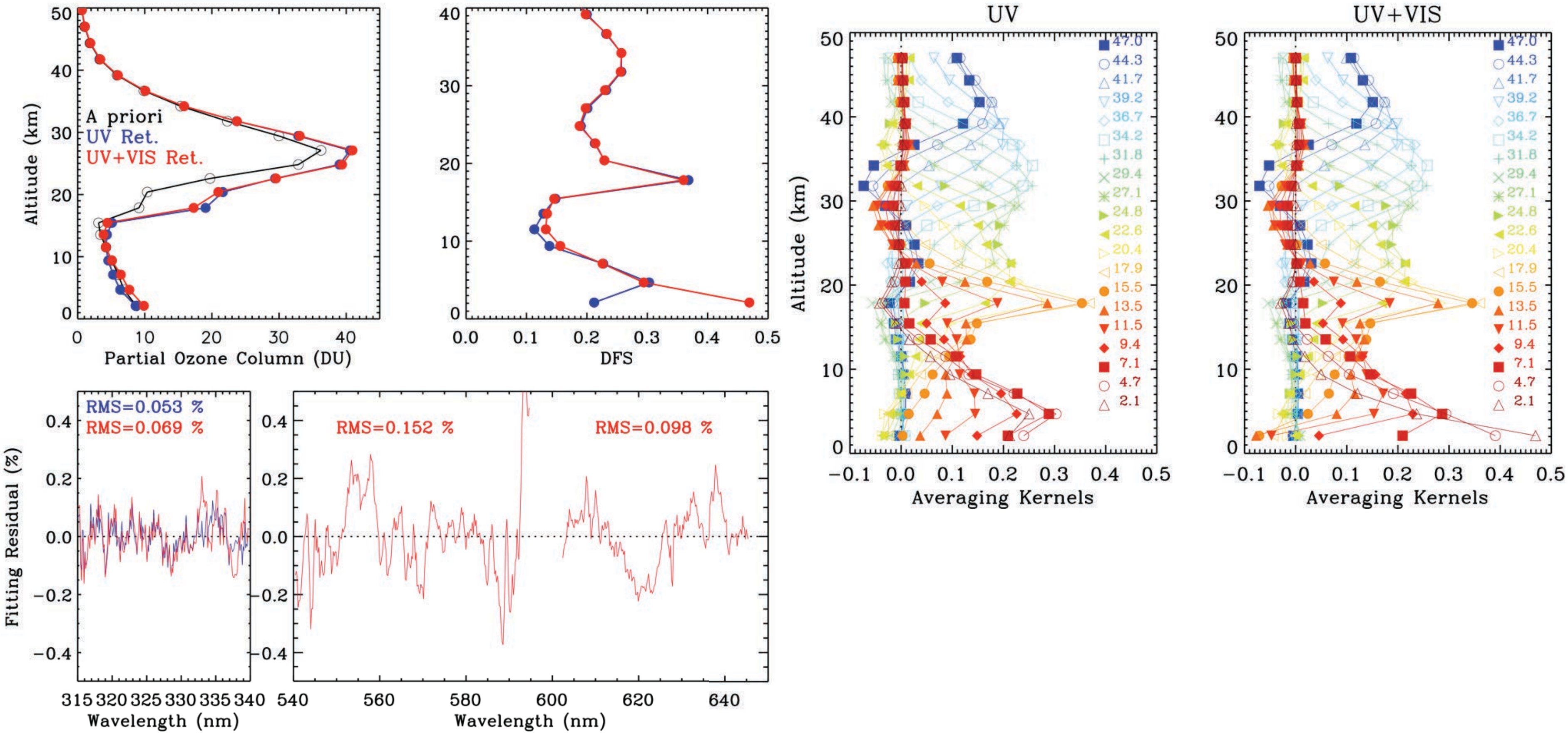
Example of Synthetic Nonlinear Retrievals: Vegetation, UV/VIS vs. UV



- **Both UV only and UV/visible retrievals show agreement with true columns to within retrieval precision.**
- **UV/visible retrievals show better agreement with true columns, smaller retrieval errors but larger retrieval precisions vs. UV retrievals all due to improved retrieval sensitivity.**

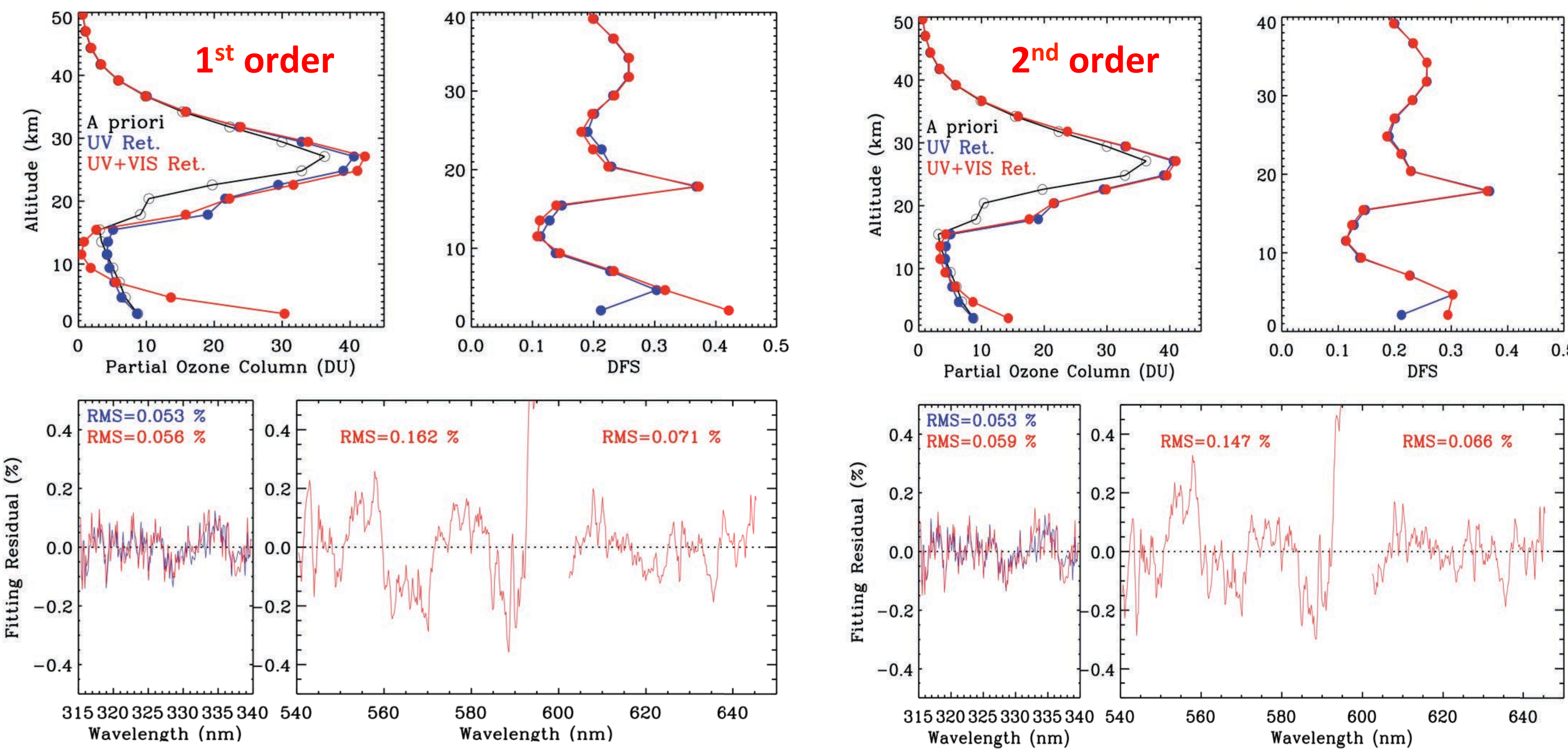
GOME-2 UV/Visible Retrievals: Impact of Visible Surface Albedo Parameters

- One pixel at: 113.2°W, 32.7°N with an effective cloud fraction of 0.08
- Fitting 2 EOFs in bands 3 & 4, respectively (4 parameters): UV+visible shows significant DFS increase mainly in the lower troposphere, but still with relatively large fitting residuals in the visible (0.1-0.15%)



GOME-2 UV/Visible Retrievals: Impact of Visible Surface Albedo Parameters

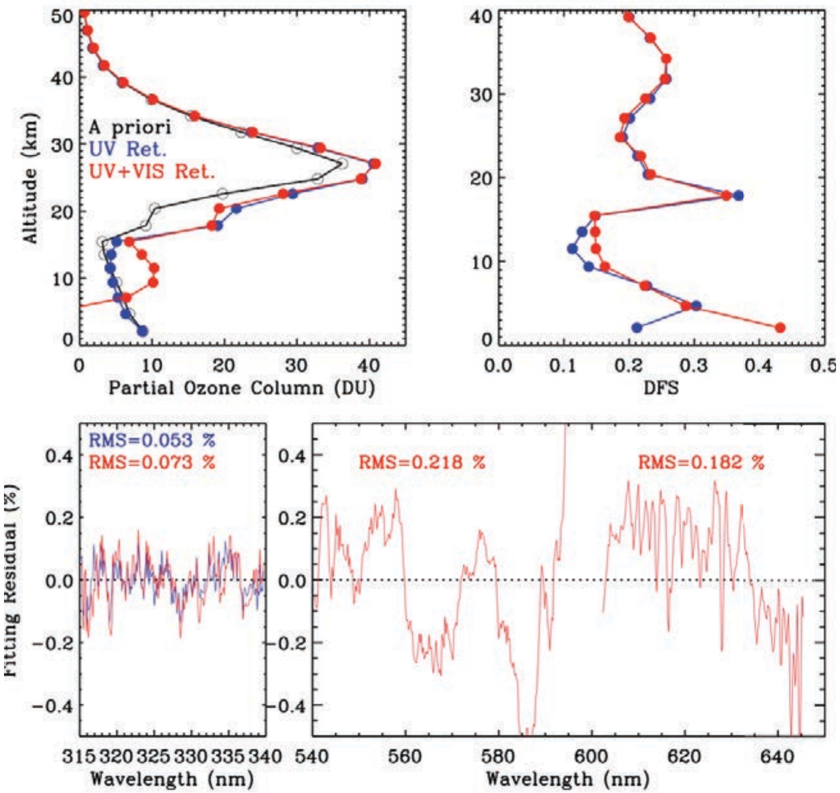
- **Scaling albedo spectra (1st & 2nd orders) in bands 3 & 4, respectively (4 & 6 parameters): more parameters leads to better fitting but also less retrieval enhancement.**



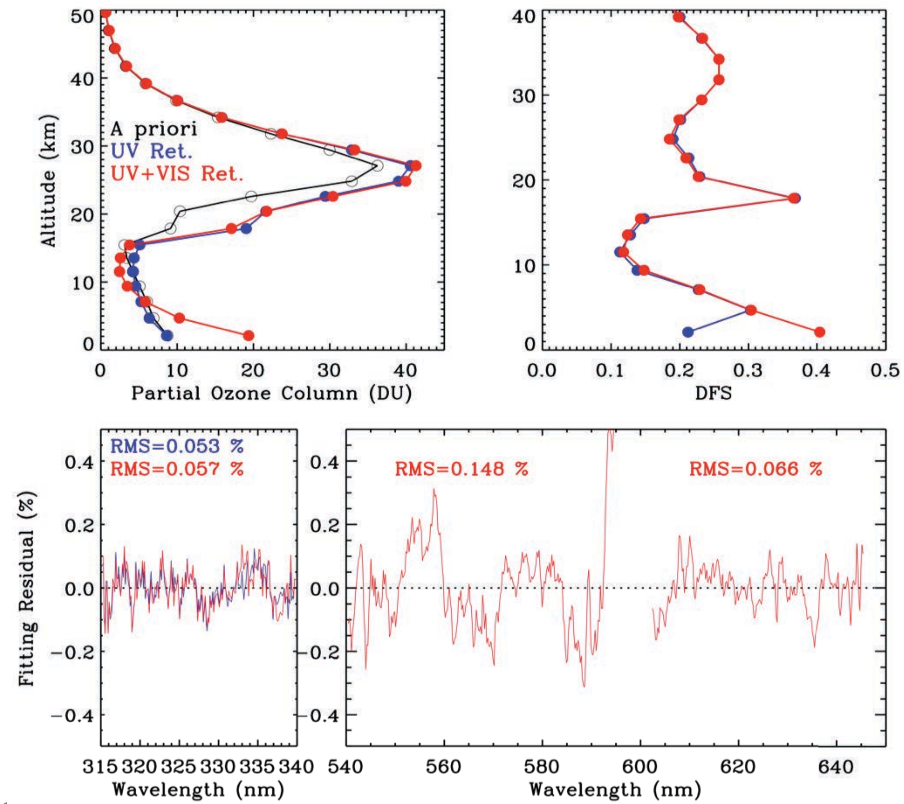
GOME-2 UV/Visible Retrievals: Impact of Visible Surface Albedo Parameters

- Scaling albedo spectra (2nd order) in visible (i.e., bands 3 + 4 together, 3 parameters): larger fitting residuals and very small tropospheric O_3 values.
- Add a scaling parameter (4 parameters) in band 4 radiance can significantly reduce fitting residuals. This suggests calibration inconsistency across channels.

2nd order in visible



2nd order in visible, I scaling in band4



GOME-2 UV/Visible Retrievals: Impact of Visible Surface Albedo Parameters

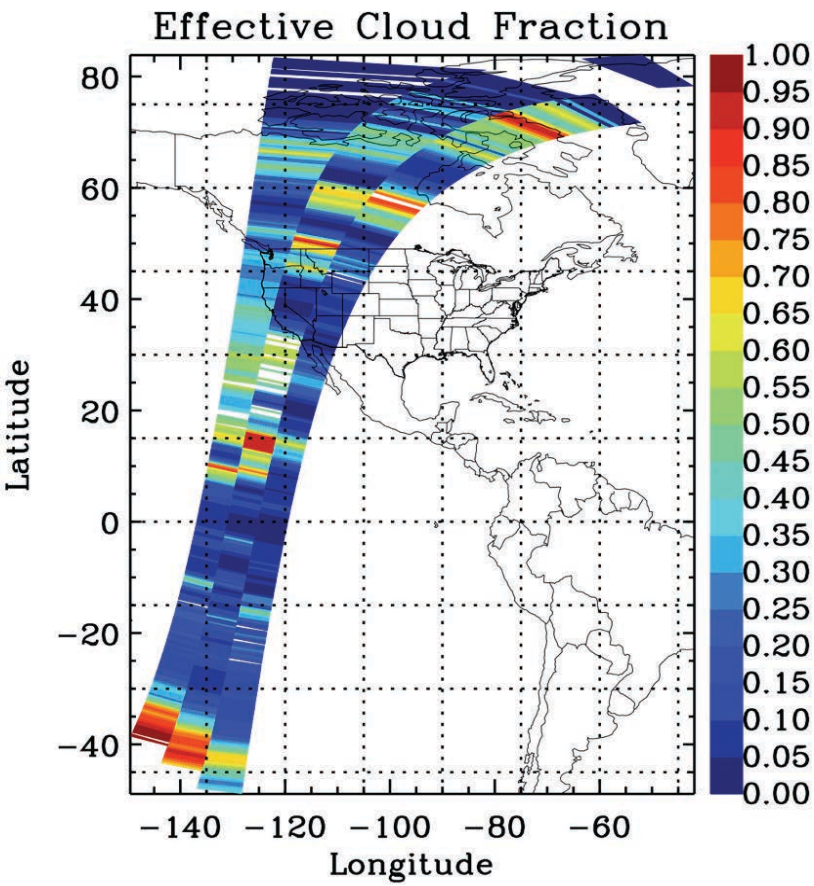
- Impact of surface albedo fitting parameters on the retrievals

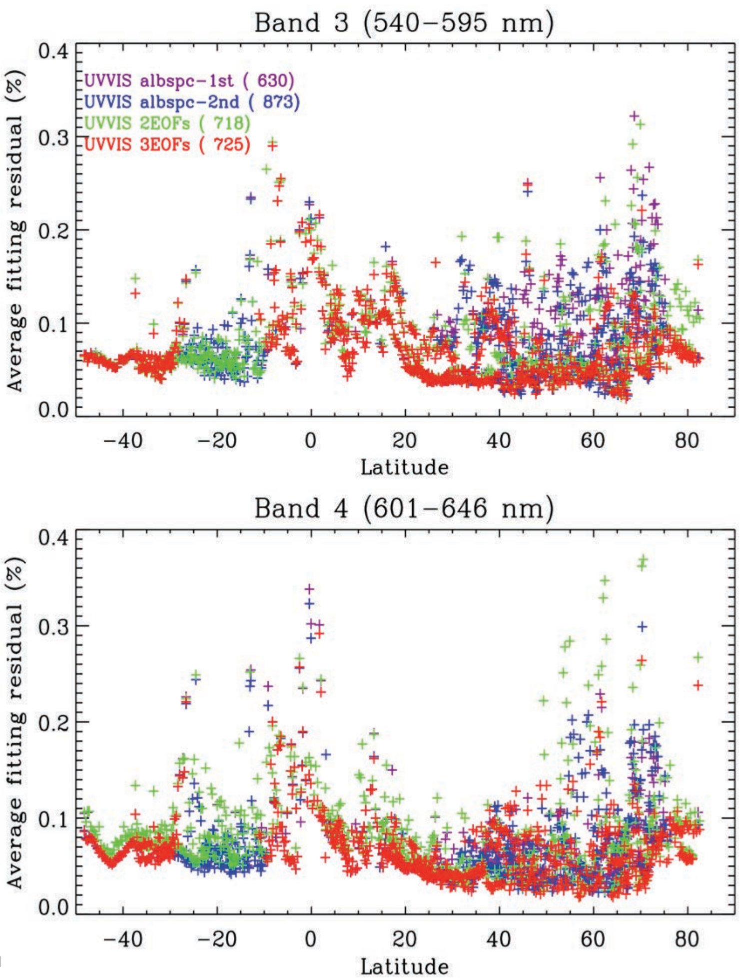
Options	Trop. DFS	TOC (DU)	Band 3 Res (%)	Band 4 Res (%)
UV	1.27	38.5		
UVVIS 2albspc, 2W	1.48	55.2	0.162	0.071
UVVIS 3albspc, 2W	1.35	44.0	0.147	0.066
UVVIS 3albspc, 1W	1.55	5.4	0.218	0.182
UVVIS 3albspc, 1W, scale band 4 rad.	1.47	47.8	0.148	0.066
UVVIS 2 EOFs, 2 W	1.56	41.6	0.152	0.098
UVVIS 3 EOFs, 2 W	1.39	47.4	0.141	0.076
UVVIS 3 EOFs, 1 W	1.83	84.9	0.217	0.160
UVVIS 3 EOFs, 1 W, scale band 4 rad.	1.82	79.9	0.138	0.100

*** 2W: band 3, 4 separately, 1W: visible (band 3+4 together)**

GOME-2 UV/Visible Retrievals

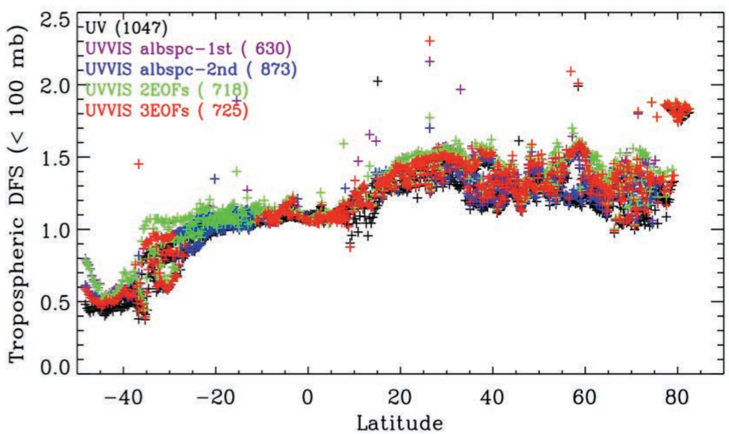
- One orbit of GOME-2 data overpass North America on 1 July 2008
- UV/visible retrievals still show frequent retrieval failures (mostly negative O_3 values or do not converge) and large band 3-4 residuals with some albedo options.

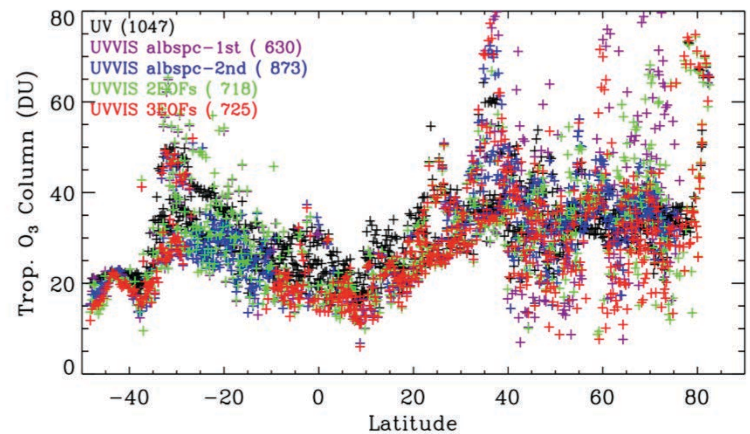


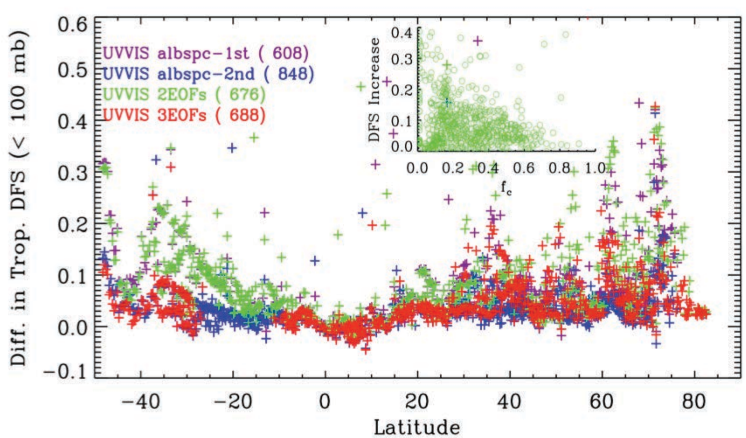


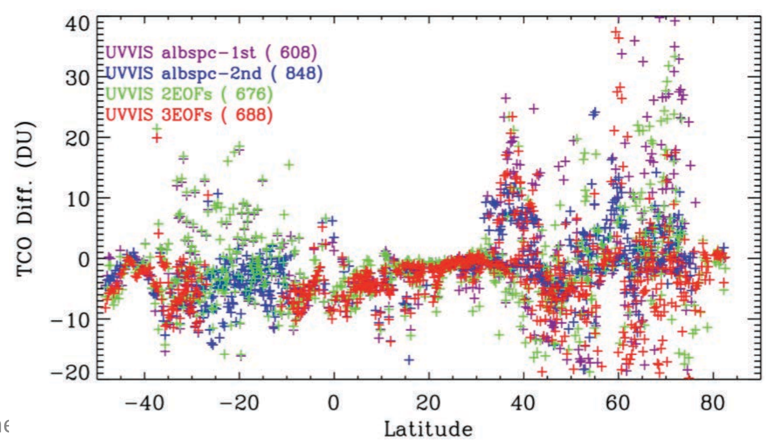
GOME-2 UV/Visible Retrievals

- Some retrievals show clearly tropospheric DFS (>100 mb) increase of up to 0.30 and significant changes in tropospheric O_3 column over land under nearly clear-sky conditions especially with 2 EOF or 1st-order scaling option.
- Fitting higher order EOFs/albedo typically improves fitting residuals, but decreases DFS and tropospheric ozone column difference.









Summary and Future Outlook

- UV only algorithm has been successfully implemented (e.g., GOME, OMI, and GOME-2, OMPS)
- Adapted our UV O_3 profile algorithm for joint UV/visible retrievals including the modeling of surface albedo spectrum
- Synthetic retrievals verify the retrieval enhancement to lower tropospheric ozone with additional visible.
- Preliminary retrievals demonstrate the potential of adding visible to improve ozone profile retrievals in the lower troposphere
- However, retrievals are very sensitive to the fitting of surface albedo parameters; relatively large fitting residuals still occur
- Near-term work to joint UV/visible retrievals will include:
  - Updated to use new version of GOME-2 data and account for provided view-angle dependent correction
  - Further improve surface albedo modeling and fitting
  - Refine the derivation of empirical calibration among different bands.
  - Account for aerosols and surface BRDF
  - Validate both UV/visible & UV only retrievals against ozonesonde observations, and examine retrievals in regions of pollution episodes.