Version 8 Ozone EDR Validation

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NOAA and NASA OMPS Teams

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Context

- The algorithms to generate the Total Column Ozone and Nadir Ozone Profile EDR estimates from the OMPS instruments are in the process of a migration from the IDPS system to the NDE system. As part of this transition, we are switching from the Multiple Triplet Algorithm (MTTOz) to the Enterprise Version 8 Total Ozone Algorithm (V8TOz).
- We have been making the OMPS V8TOz and OMPS V8Pro products offline for the last four years and tracking their performance as the OMPS Nadir Mapper and Nadir Profiler SDR processing has introduced improvements and new calibration characterizations. See www.star.nesdis.noaa.gov/smcd/spb/OMPSDemo/proOMPSbeta.TOZ_V8.php
- We work with the NASA OMPS Science Team, the OMPS SDR Team, and ozone researchers at NCEP and ESRL.
- The Total Ozone and Nadir Ozone Profile EDRs are part of the suite of data products from the JPSS system. These particular products are used to monitor the ozone layer and as input to NWMs. In particular, the UV Index forecast product requires good quality maps of total column ozone.
- JPSS has been providing funding for all aspects of this work including product validation and code transition. Funding was provided by NCDC for the initial implementation of the V8TOz and V8Pro for OMPS at NOAA.

Challenges

- The SDR advances and improvements have presented a moving target for validation. We do not have sufficient resources for full SDR reprocessing after each change, so new comparisons must be generated over time following major SDR changes.
- The V8TOz was delivered last year for implementation at IDPS but the program redirected the implementation to NDE. We completed the S-NPP V8TOz ARR and DAP last month and are nearing completion of a refinement for J-01 processing to address degradation in the retrievals due to elevated atmospheric SO_2 levels.
- The V8Pro has been delivered and implemented at IDPS but we have been instructed to move it to NDE as well. The code is awaiting a security review and will be delivered after we hold an Algorithm Readiness Review.
- Estimates of precision require characterization of uncertainties in the retrievals due to profile shapes and ozone below clouds. The truth conditions are difficult to verify for individual measurements due to matchup and validation data set uncertainties. We have used various difference techniques to use the data itself to estimate these uncertainties.

Actions

- The V8TOz and V8Pro algorithms are well-designed with excellent suites of measurement residuals and response efficiencies to relate uncertainties in products to uncertainties in measurements or intermediate products.
- The content has been refined and exercised over the last 40 years by a sequence of NASA Science Teams. They have empirically-tuned adjustments for UV absorbing aerosols, sun glint and profile shape variations and improved RT model information on inelastic scattering.
- The algorithms use extensive sets of satellite and ground-based measurements to provide standard and a priori ozone and temperature profiles and cloud top pressure for use with UV measurements.

Results

- The V8TOz DAP has been delivered to NDE. The V8Pro is awaiting code and algorithm readiness reviews. The implementation at NDE will be this fall after the end of the Block 2.0 ORR freeze. The V8TOz and V8Pro operate on single granules of OMPS NM and NP SDR and GEO.
- The V8TOz is used to generate the NOAA Operational GOME-2 total ozone products and the NASA EOS Aura OMI total ozone product.
- The V8Pro is used to generate the NOAA Operational SBUV/2 ozone profile products.
- Papers in JGR on OMPS SDR and EDRs
  - Seftor et al. [2014] doi:10.1002/2013JD020472
  - Wu et al. [2014] doi:10.1002/2013JD020484
  - Flynn et al. [2014] doi:10.1002/2013JD020467
  - Jaross et al. [2014] doi:10.1002/2013JD020482
- Other References
  - Bhartia et al., (2013) SBUV total ozone and profile algorithm; doi:10.5194/amt-6-2533-2013.
  - Wellemeyer, C. G., et al., (1997), A correction for total ozone mapping spectrometer profile shape errors at high latitude, J. Geophys. Res., 102(D7), 9029–9038, doi:10.1029/96JD03965.

Future Plans

- We will evaluate the V8TOz and V8Pro products once they are at NDE and make sure that they show the same performance as our offline products. We will use them to populate the ICVS monitoring pages instead of the offline products currently monitored there.
- A presentation will be given to the SPSRB when the products are ready for operational distribution from NDE.
- We are providing our ICVS product monitoring tools to OSPO. They will use some of these and also replicate their existing SBUV/2 and GOME-2 monitoring.
- The exclusion for elevated SO_2 amounts (> 6 DU) goes away for J-01. We are preparing to hold a delta Algorithm Readiness Review and deliver the $LFSO_2$ algorithm to NDE. This algorithm uses the V8TOz measurement residuals to make an estimate of the atmospheric SO_2, and then uses this SO_2 estimate to correct the total column ozone estimate.
- The codes delivered to NDE are ready to process the medium resolution OMPS SDRs planned for the JPSS-01 operations.

OMPS Total Ozone Product Requirements

- JPSS Level 1 Requirements Document (L1RD) Supplement for the OMPS Ozone Total Column Environmental Data Records (EDRs)

Table 5.2.11 - Ozone Total Column (O

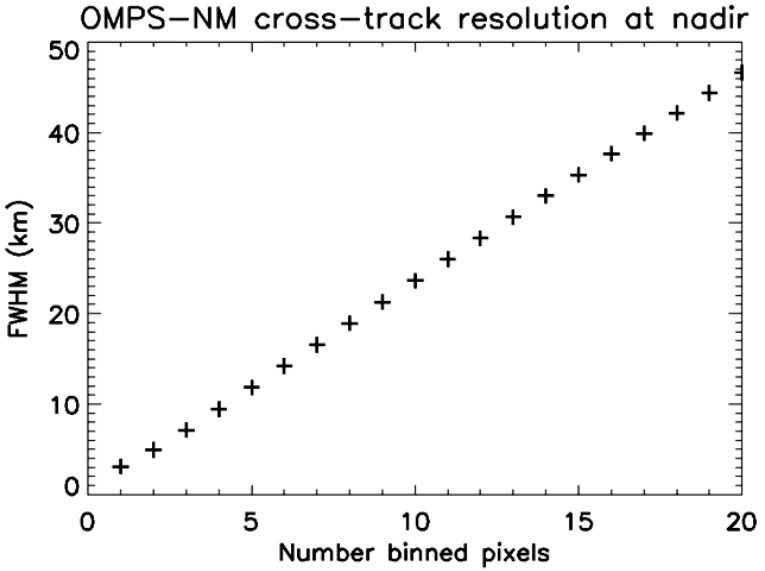
EDR Attribute	Threshold
Ozone TC Applicable Conditions: 1. Threshold requirements only apply under daytime conditions with Solar Zenith Angles (SZA) up to 80 degrees. 2. The EDR shall be delivered for all SZA.	
a. Horizontal Cell Size	50 x 50 km^2 @ nadir
b. Vertical Cell Size	0 - 60 km
c. Mapping Uncertainty, 1 Sigma	5 km at Nadir
d. Measurement Range	50 - 650 milli-atm-cm
e. Measurement Precision	
1. X < 0.25 atm-cm	6.0 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	7.7 milli-atm-cm ~2%
3. X > 0.45 atm-cm	2.8 milli-atm-cm + 1.1%
f. Measurement Accuracy	
1. X < 0.25 atm-cm	9.5 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	13.0 milli-atm-cm ~3%
3. X > 0.45 atm-cm	16.0 milli-atm-cm
g. Refresh	At least 90% coverage of the globe every 24 hours (monthly average)

Verification of Performance:

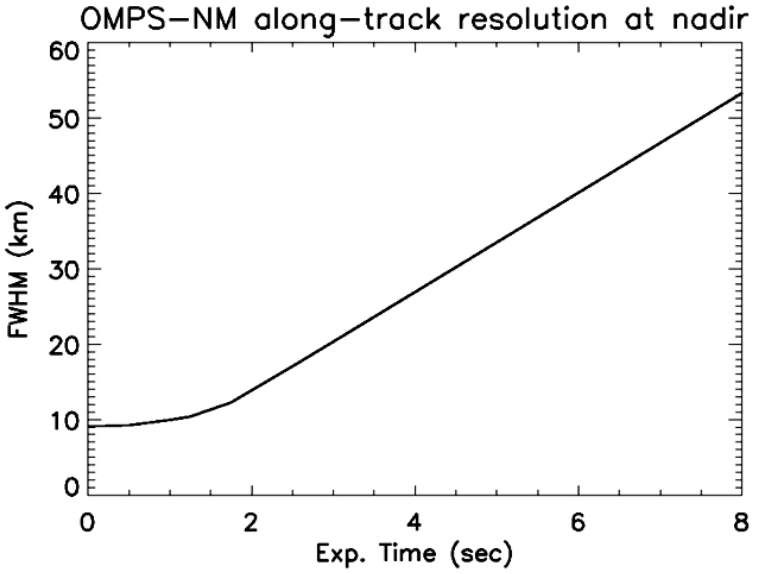
a. 20-Pixel Aggregation and 7-S along track integration.
b. 318 nm channel BUV comes from the surface to top of atmosphere. Standard profiles in tables account for full range.
c. Confirmed by coastlines and comparison to 750x750 m^2 VIIRS.
d. Confirmed by standard profiles and four years of processing and ground-based matchup scatter.
e. Precision estimates from Nearest Neighbor analysis. Use of 1512 Latitude/Month/TOz profiles.
f. Accuracy is adjusted by soft calibration and checked by zonal mean and overpass statistics.
g. 105° cross-track swath provides full daily coverage.

(a) Horizontal Cell Size
Flight Parameters and Lab MTF

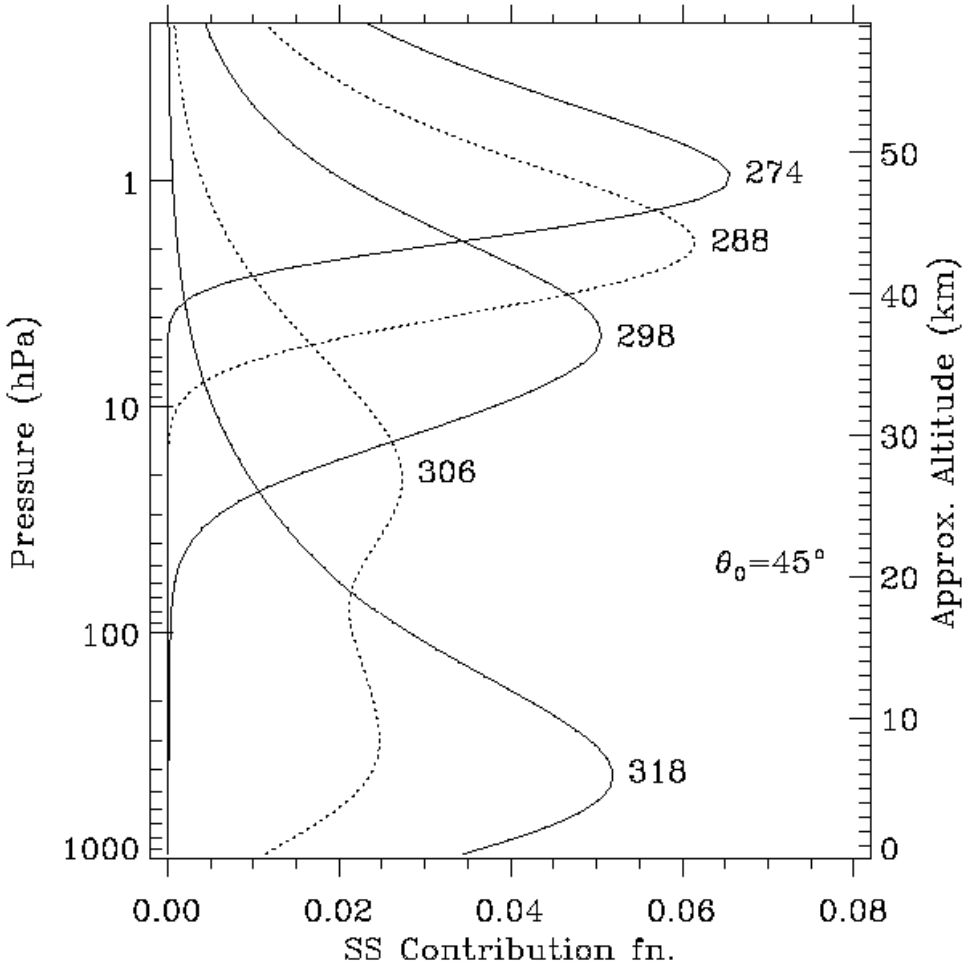
- Across-Track
  - 20 pixels at 2.5 km/pixel
  - = 50 km

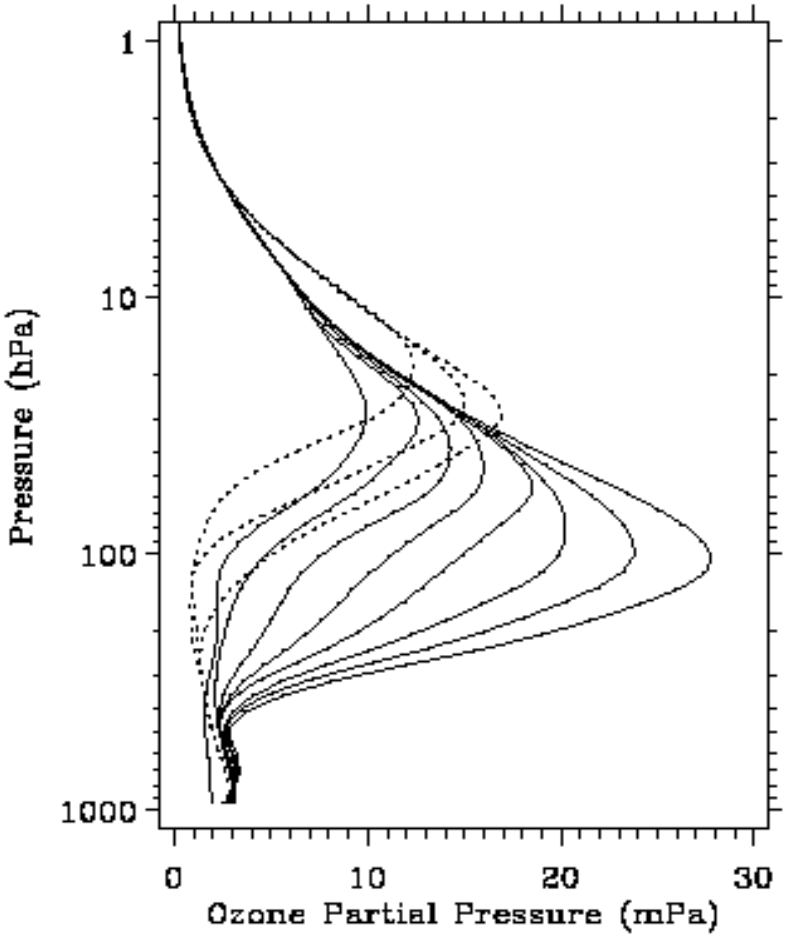


- Along-Track
  - 7.5 S integration at 6.56 km/S
  - = 49.2 km motion

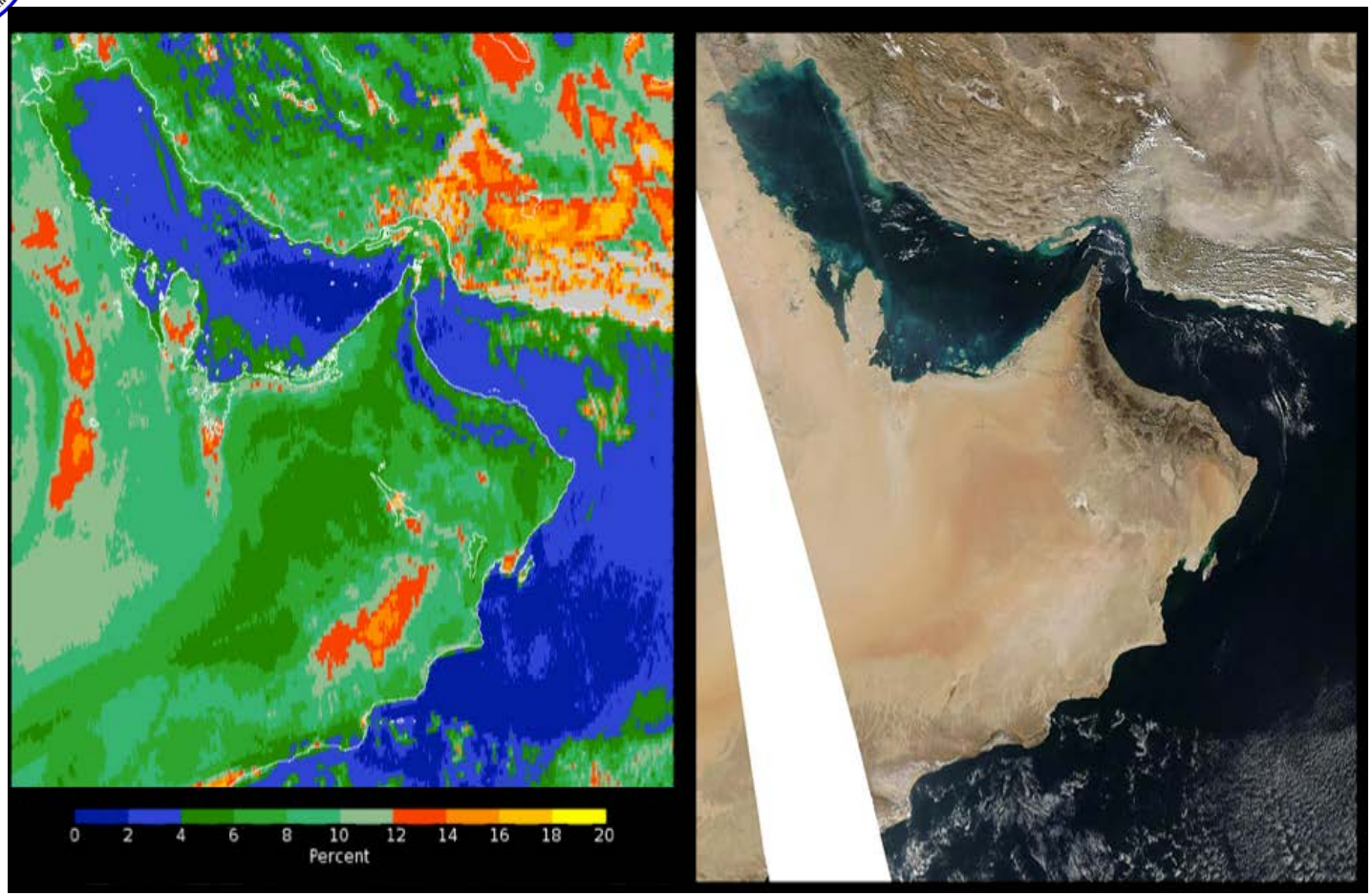


(b) 318 nm Contribution Function and Standard Ozone Profiles

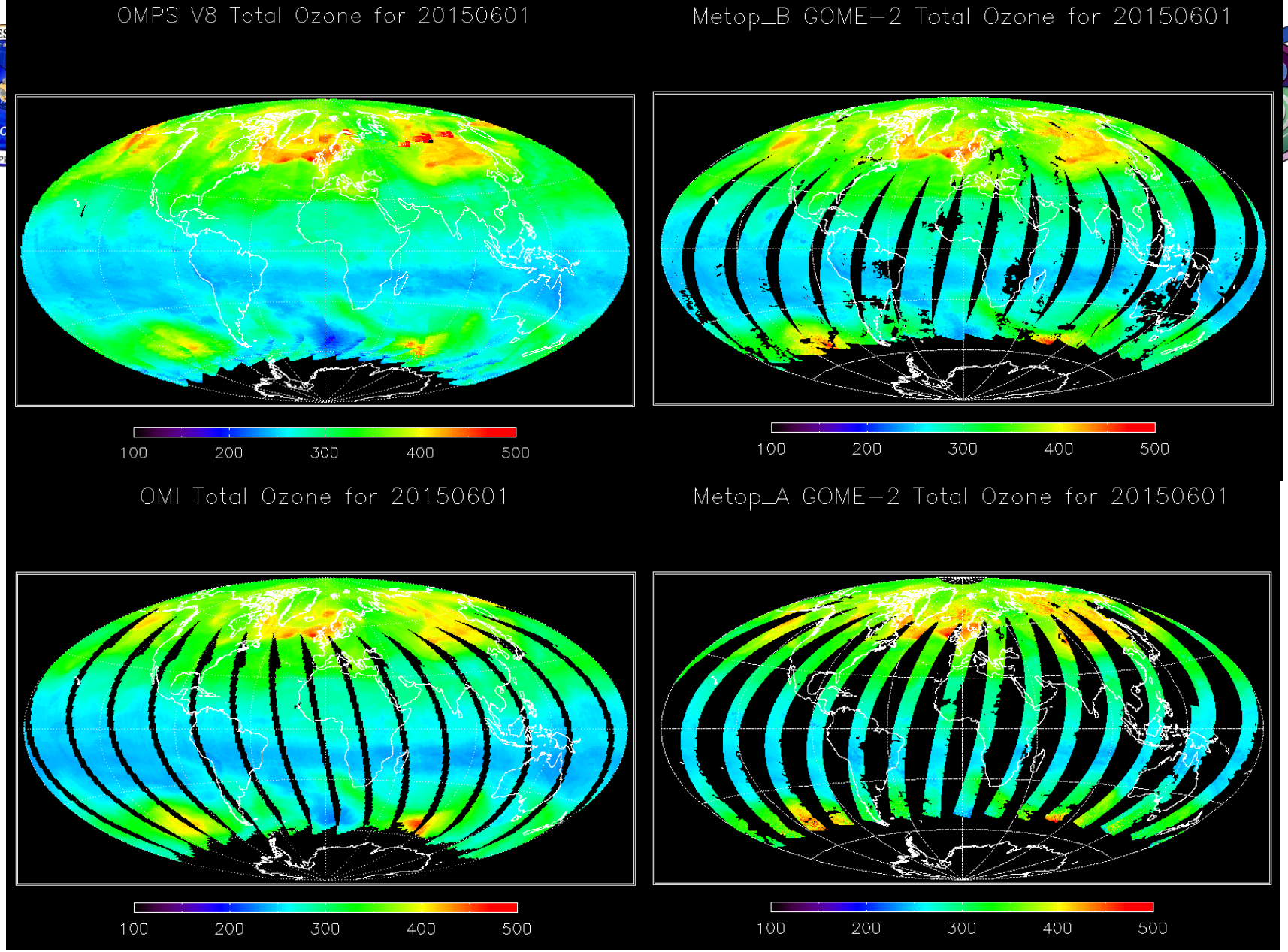




(c) Geolocation Uncertainty

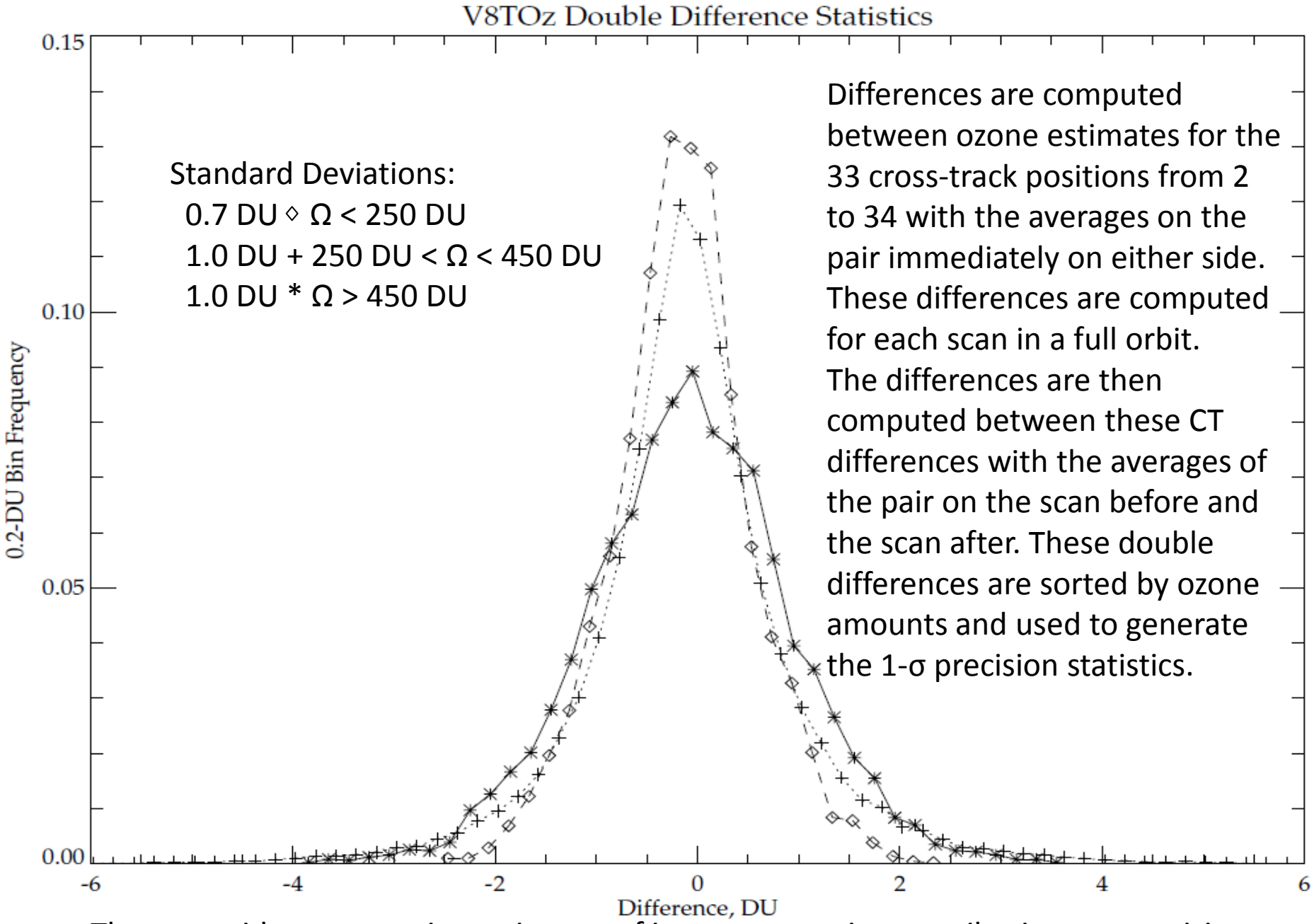


High-Spatial-Resolution for Geolocation. The image on the left shows a false color map of the OMPS effective reflectivity (from a single Ultraviolet channel at 380 nm) over the Arabian Peninsula region for January 30, 2012 when the instrument was making a set of high-spatial-resolution measurements with 5×10 km^2 FOVs at nadir. The color scale intervals range from 0 to 2% in dark blue to 18 to 20% in yellow. The image on the right is an Aqua Moderate Resolution Imaging Spectroradiometer (MODIS) Red-Green-Blue image for the same day. (Provided by C. Seftor, SSAI.)



(g) Refresh, (d) Range and (f) Accuracy from Daily maps of total column ozone.
The false color maps show the total column ozone in Dobson Units for June 1, 2015 for the V8TOz algorithm applied to S-NPP OMPS (Top Left), Metop-B GOME-2 (Top Right), EOS Aura (Bottom Left) and Metop-A GOME-2 (Bottom Right).

(e) Measurement Precision



Standard Deviations:
0.7 DU ◊ Ω < 250 DU
1.0 DU + 250 DU < Ω < 450 DU
1.0 DU * Ω > 450 DU

Differences are computed between ozone estimates for the 33 cross-track positions from 2 to 34 with the averages on the pair immediately on either side. These differences are computed for each scan in a full orbit. The differences are then computed between these CT differences with the averages of the pair on the scan before and the scan after. These double differences are sorted by ozone amounts and used to generate the 1-σ precision statistics.

These provide conservative estimates of instrument noise contributions to precision.

Using V8TOz dN/dR and dN/dO3 to determine soft calibration adjustments

The V8TOz output contains a variety of useful parameters in addition to the total column ozone estimates. In particular, the retrieval sensitivities, dy/dx can be used to give soft calibration estimates of the N-value changes to remove reflectivity and ozone bias. If you want to increase the effective reflectivity, R, and the total column ozone, Ω, by ΔR and ΔΩ then you should increase the N-values by

$$\Delta N318 = \Delta R\ dN318/dR + \Delta\Omega\ dN318/d\Omega = \Delta R\ A1 + \Delta\Omega\ B1$$

$$\Delta N331 = \Delta R\ dN331/dR + \Delta\Omega\ dN331/d\Omega = \Delta R\ A2 + \Delta\Omega\ B2$$

where dNw/dR is the rate of change of the N-value, Nw, for wavelength, w, with respect to changes in the effective reflectivity, R, and dNw/dΩ is the rate of change of the N-value, Nw, for wavelength, w, with respect to changes in the total column ozone, Ω.

Conversely, if you increase the N values by C1=ΔN318 and C2=ΔN331, then the retrieved R and Ω increase by

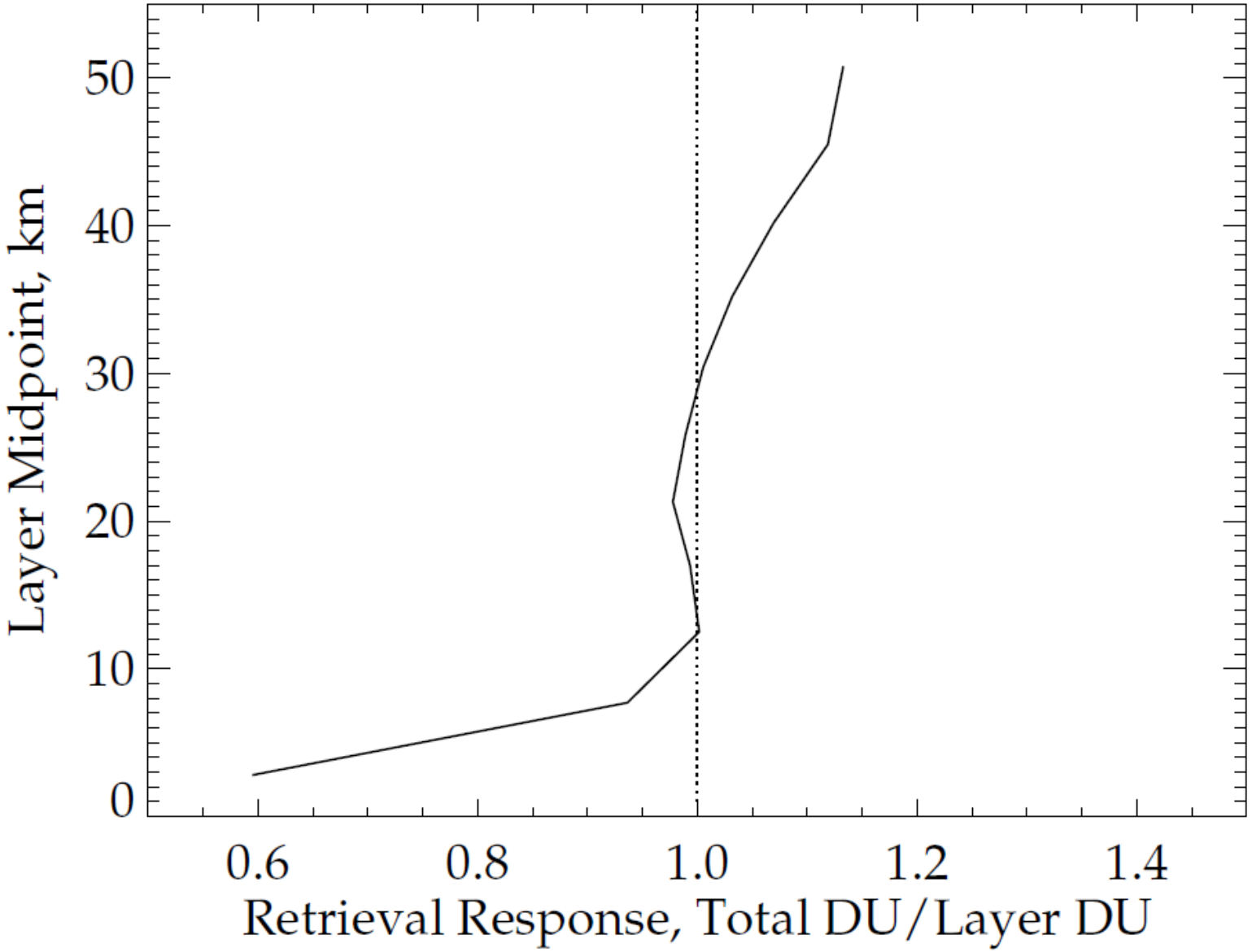
$$\Delta R = [C1 * dN331/d\Omega - C2 * dN318/d\Omega] / D$$

$$\Delta\Omega = -[C1 * dN331/dR, - C2 * dN318/dR] / D$$

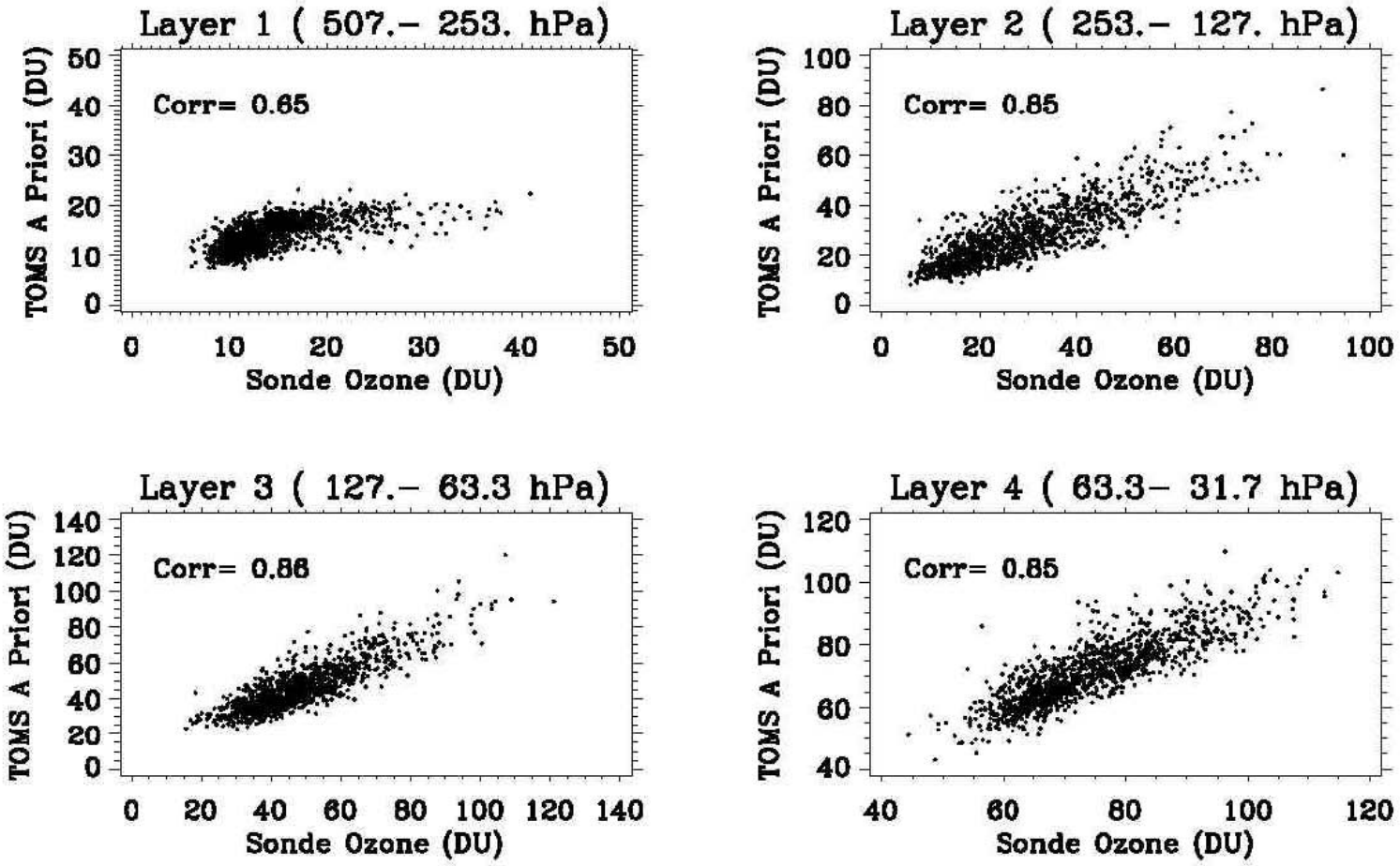
$$D = [dN318/dR * dN331/d\Omega - dN331/dR * dN318/d\Omega]$$

Ω is total ozone in DU, R is effective reflectivity, and N is -100*log10(Radiance/Irradiance)

Total Ozone Retrieval Efficiency



Errors from Tropospheric Variations



Comparisons between Hohenpeissenberg ozonesonde layer amounts and the 96 standard profiles in the 3-dimensional set used at its latitude.

Comparison of *A Priori* profiles with ozonesonde and SAGE

Layer (No.)	Layer midpoint (~km)	Hohenpeissenberg		SAGE @50°N	
		Variance reduction (%)	Residual std dev (DU)	Variance reduction (%)	Residual std dev (DU)
0	2.8	41	2.9	-	-
1	7.7	42	3.8	-	-
2	12.5	73	7.6	75	9.7
3	17.0	74	7.4	83	8.9
4	21.3	73	6.0	77	6.4
5	25.8	24	5.5	29	5.3
6	30.4	42	3.5	35	4.3
7	35.2	-	-	39	1.9
8	40.2	-	-	28	1.0
9	45.5	-	-	40	0.5

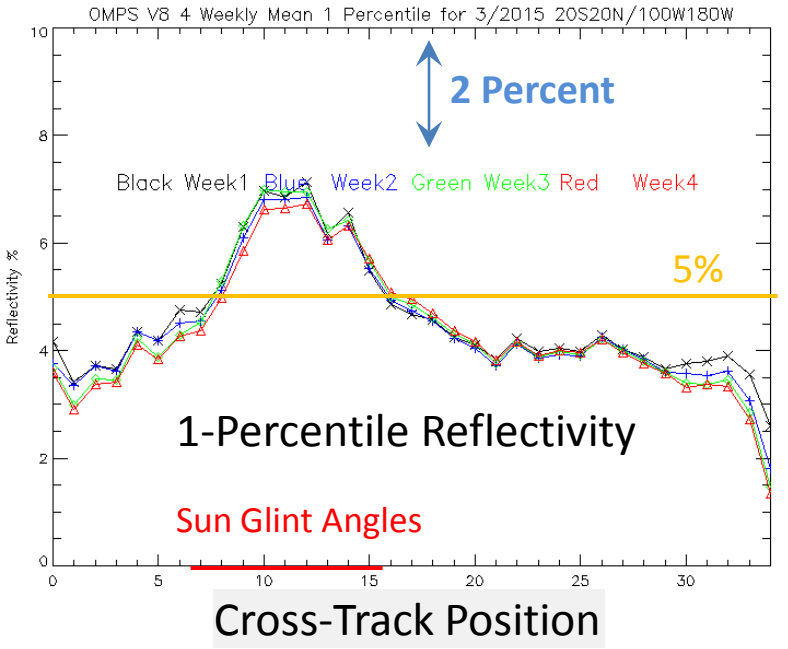
Offline Processing at STAR

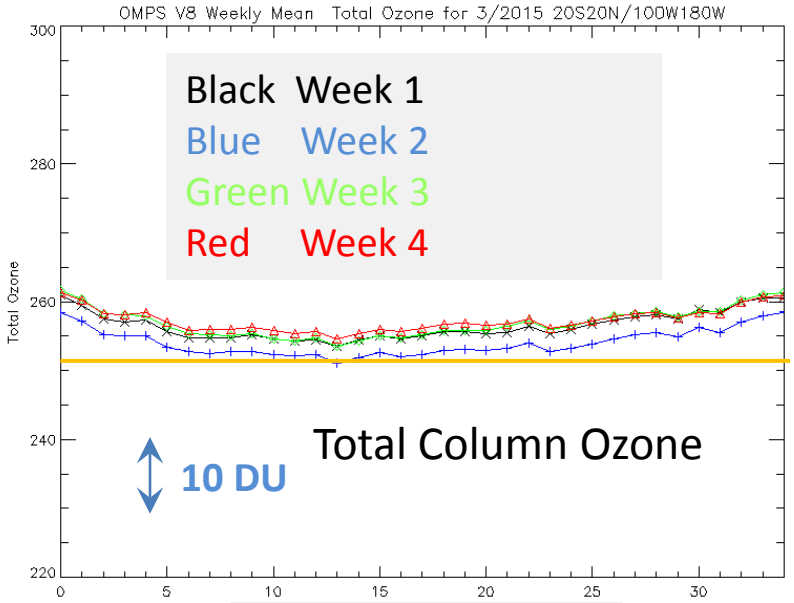
- The V8TOz has been used to process the first four years of OMPS NM SDRs to produce full daily global maps on the LINUX system at STAR.
- The products from this processing have been monitored and validated with a suite of analysis and comparison figures available at

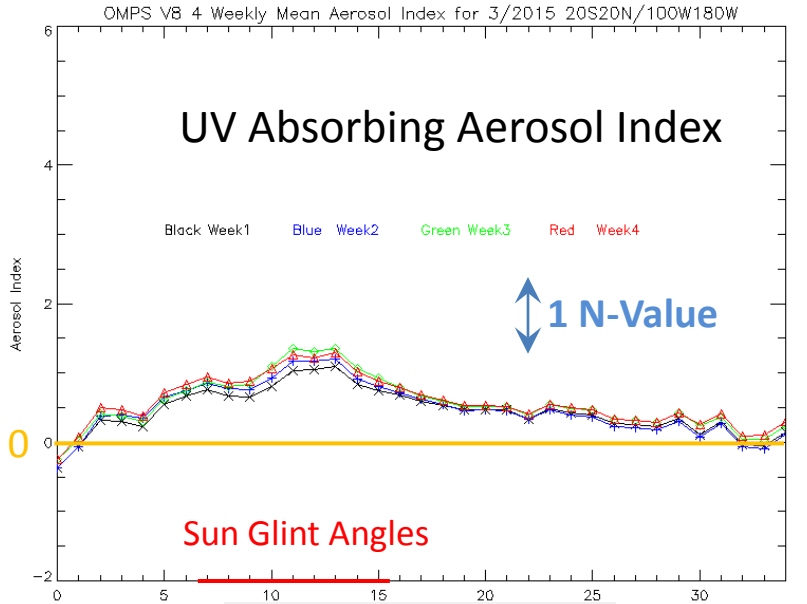
  www.star.nesdis.noaa.gov/smcd/spb/OMPSDemo/proOMPSbeta.TOZ_V8.php
- Select figures and results are presented in the following slides

Internal Consistency

Weekly Total Ozone, 1-percentile Effective Reflectivity and Aerosol Index values, for March 2015 for a latitude / longitude box in the Equatorial Pacific versus cross-track pixel. Internal Consistency and Vicarious Calibration / Validation Generation of soft calibration coefficients (CFE) – Can use Minimum Reflectivity = 4.5%, no aerosols, no SO2, and Ozone set to EOS OMI mean.



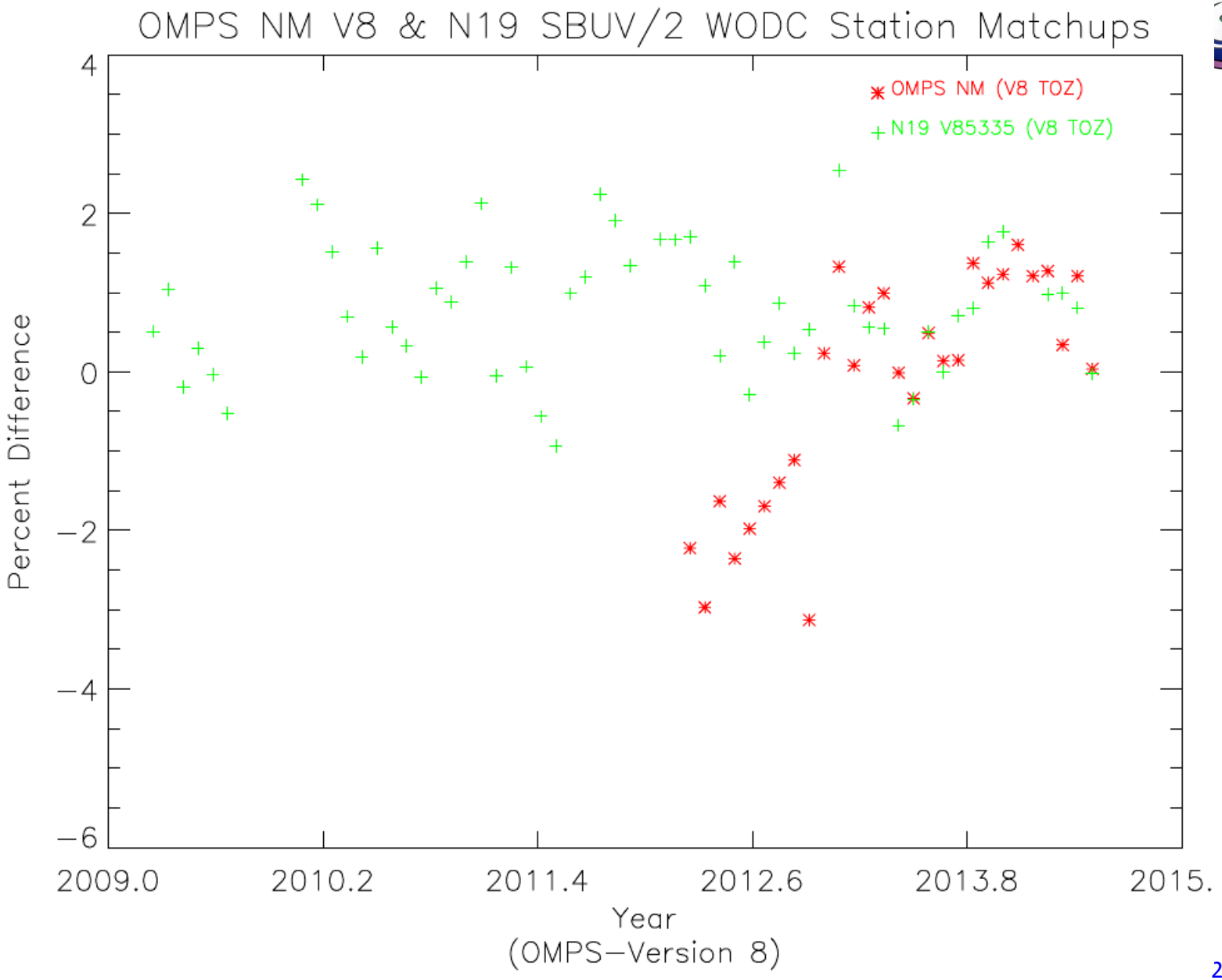




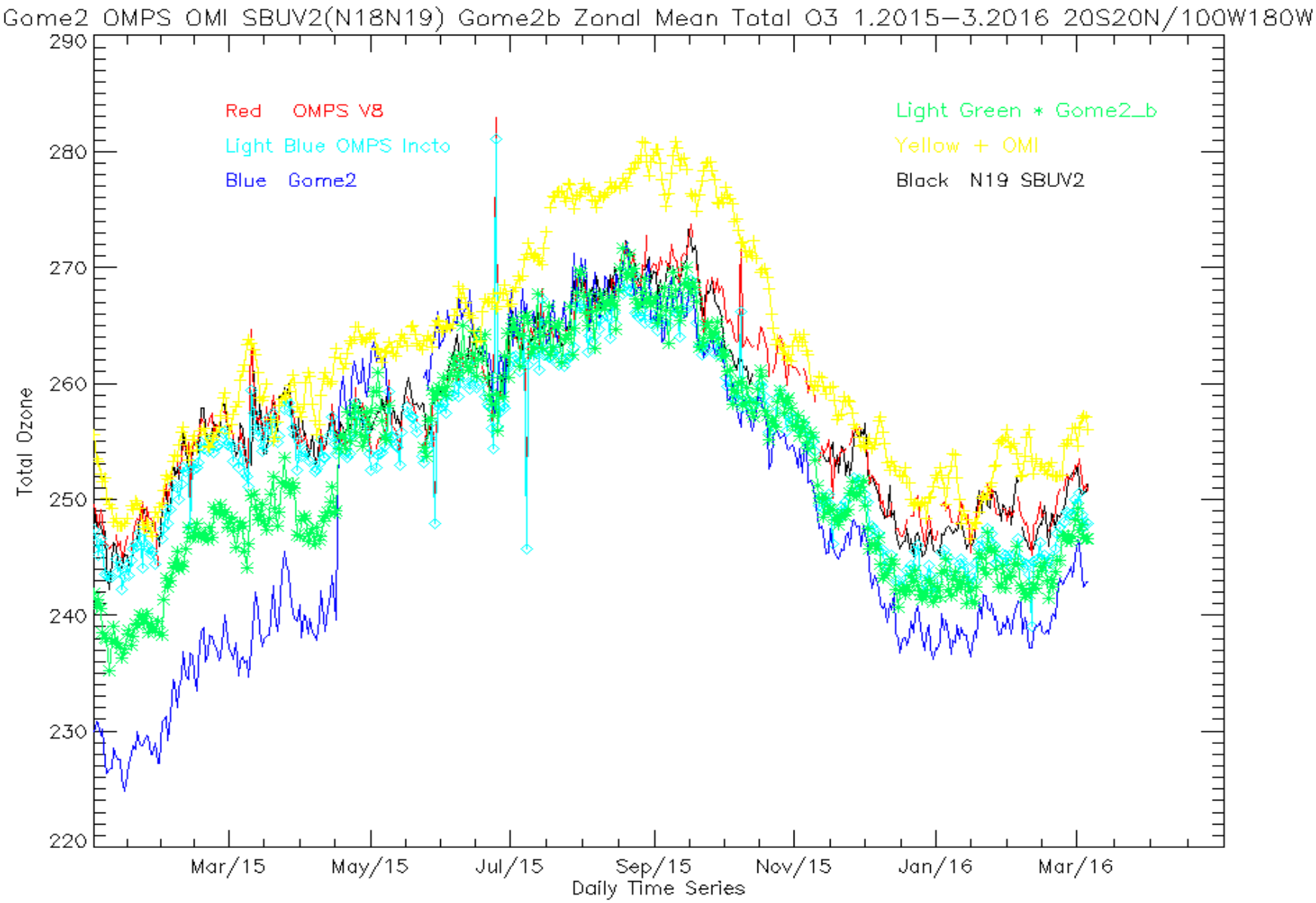
(f) Validation Data Sets

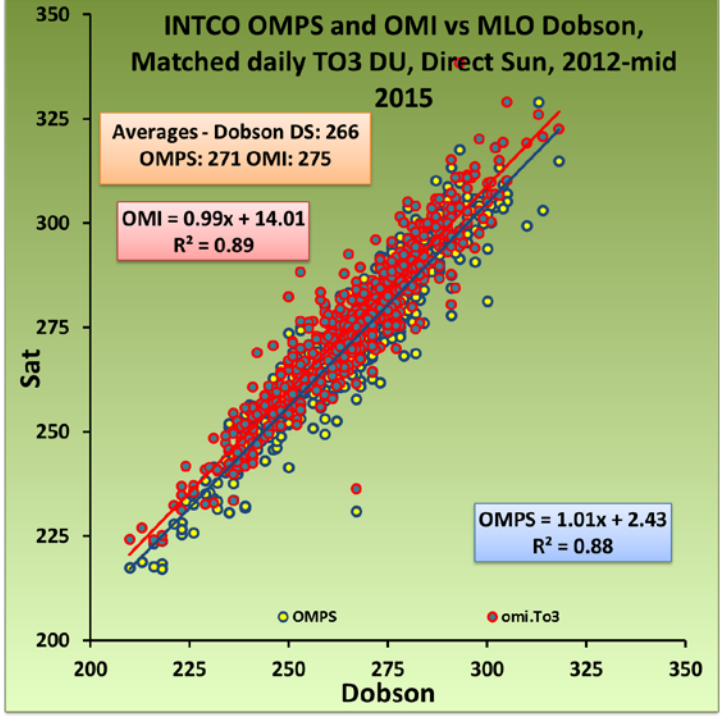
- Satellite Ozone Products
  - OMI V8TOz
  - GOME-2 V8TOz
  - MLS Ozone Profiles
- Ground-based
  - Dobson Stations total ozone
  - Umkehr Stations ozone profiles
  - Balloon sondes

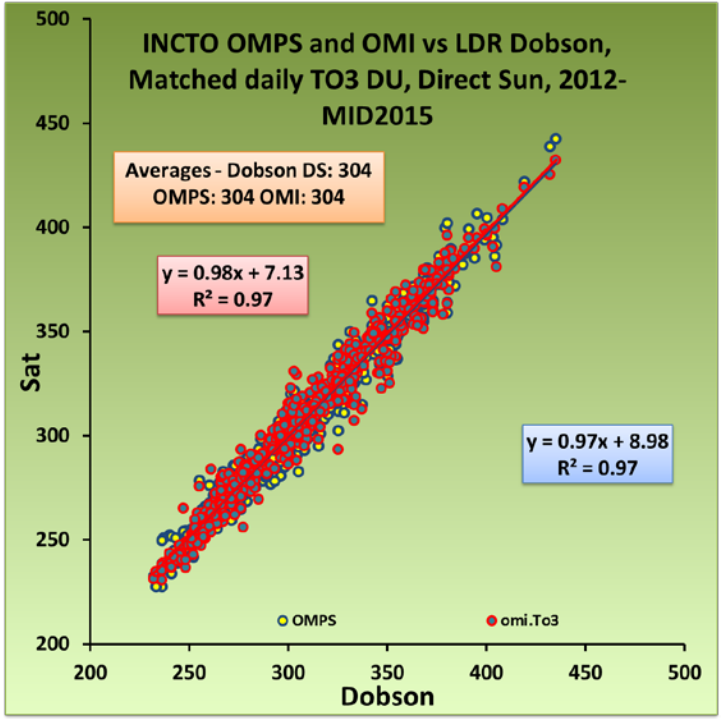
(f) Comparison to 23 Dobson Stations

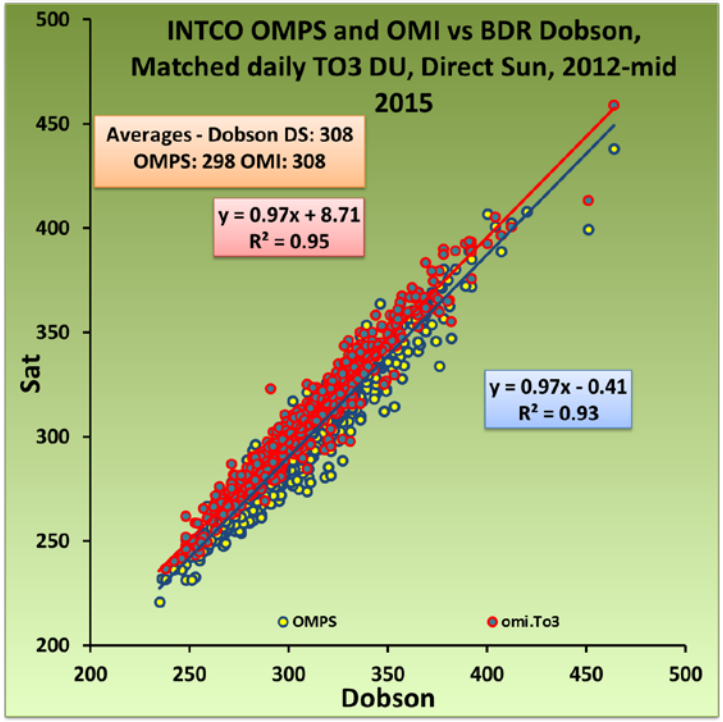


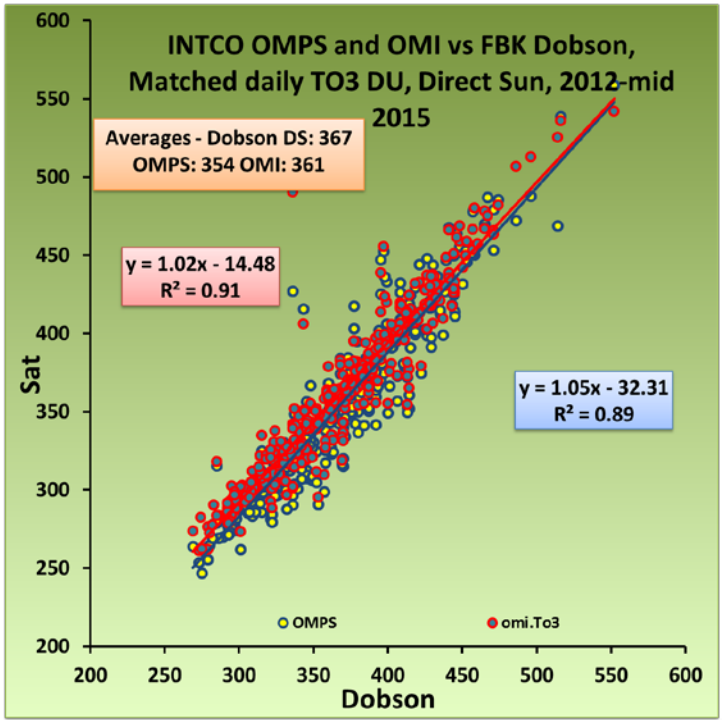
(f) Comparisons to other Satellites




INTCO OMPS and OMI vs MLO Dobson, Matched daily TO3 DU, Direct Sun, 2012-mid 2015
Averages - Dobson DS: 266
OMPS: 271 OMI: 275
OMI = 0.99x + 14.01
R² = 0.89
OMPS = 1.01x + 2.43
R² = 0.88
OMPS
omi.To3
Sat
Dobson
200
225
250
275
300
325
350


INCTO OMPS and OMI vs LDR Dobson, Matched daily TO3 DU, Direct Sun, 2012-MID2015
Averages - Dobson DS: 304
OMPS: 304 OMI: 304
y = 0.98x + 7.13
R² = 0.97
y = 0.97x + 8.98
R² = 0.97
OMPS
omi.To3
Sat
Dobson
200
250
300
350
400
450
500


INTCO OMPS and OMI vs BDR Dobson, Matched daily TO3 DU, Direct Sun, 2012-mid 2015
Averages - Dobson DS: 308
OMPS: 298 OMI: 308
y = 0.97x + 8.71
R² = 0.95
y = 0.97x - 0.41
R² = 0.93
OMPS
omi.To3
Sat
Dobson
200
250
300
350
400
450
500


INTCO OMPS and OMI vs FBK Dobson, Matched daily TO3 DU, Direct Sun, 2012-mid 2015
Averages - Dobson DS: 367
OMPS: 354 OMI: 361
y = 1.02x - 14.48
R² = 0.91
y = 1.05x - 32.31
R² = 0.89
OMPS
omi.To3
Sat
Dobson
200
250
300
350
400
450
500
550
600

V8 Total Ozone Summary

- The heritage, enterprise Version 8 Total Ozone algorithm has been delivered for implementation at NDE as part of the redirected EDR processing for JPSS.
- The EDRs from the algorithm meet the required performance levels for the Total Column Ozone when applied to the validated OMPS NM SDRs.

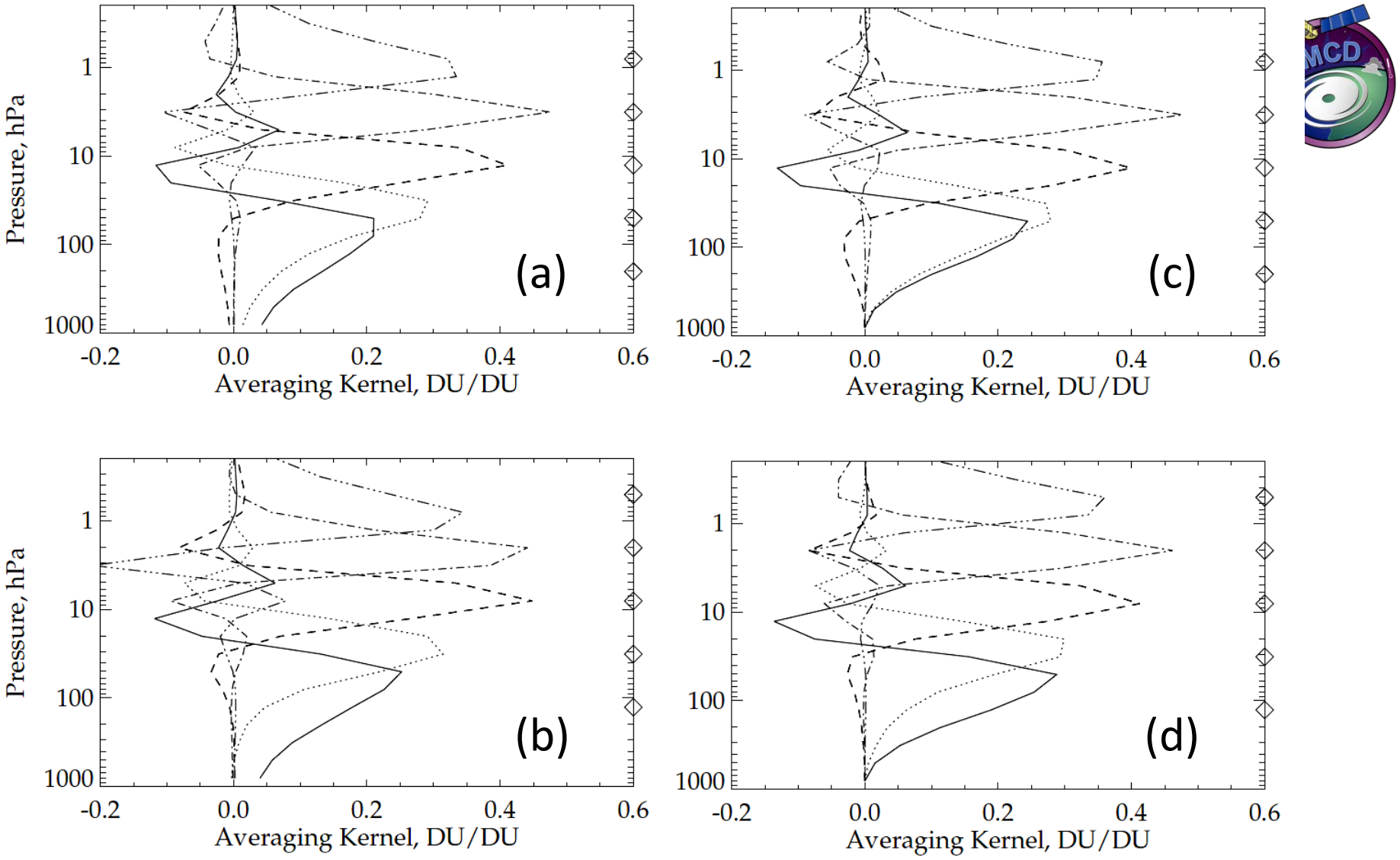
OMPS Version 8 Ozone Profile EDR Requirements

Ozone Nadir Profile (OMPS-NP) (3)	
Attribute	**Threshold**
a. Horizontal Cell Size	250 x 250 km^2 (1)
b. Vertical Cell Size	3 km reporting
1. Below 30 hPa (~ < 25 km)	10 -20 km
2. 30 -1 hPa (~ 25 -50 km)	7 -10 km
3. Above 1 hPa (~ > 50 km)	10 -20 km
c. Mapping Uncertainty, 1 Sigma	< 25 km
d. Measurement Range 0-60 km	0.1-15.0 ppmv
e. Measurement Precision (2)	
1. Below 30 hPa (~ < 25 km)	Greater of 20 % or 0.1 ppmv
2. 30 -1 hPa (~ 25 -50 km)	5% -10%
3. Above 1 hPa (~ > 50 km)	Greater of 10% or 0.1 ppmv
f. Measurement Accuracy (2)	
1. Below 30 hPa (~ < 25 km)	Greater of 10 % or 0.1 ppmv
2. 30 -1 hPa (~ 25 -50 km)	5% -10%
3. Above 1 hPa (~ > 50 km)	Greater of 10 % or 0.1 ppmv
g. Refresh	At least 60% coverage of the globe every 7 days (monthly average) (2,3)

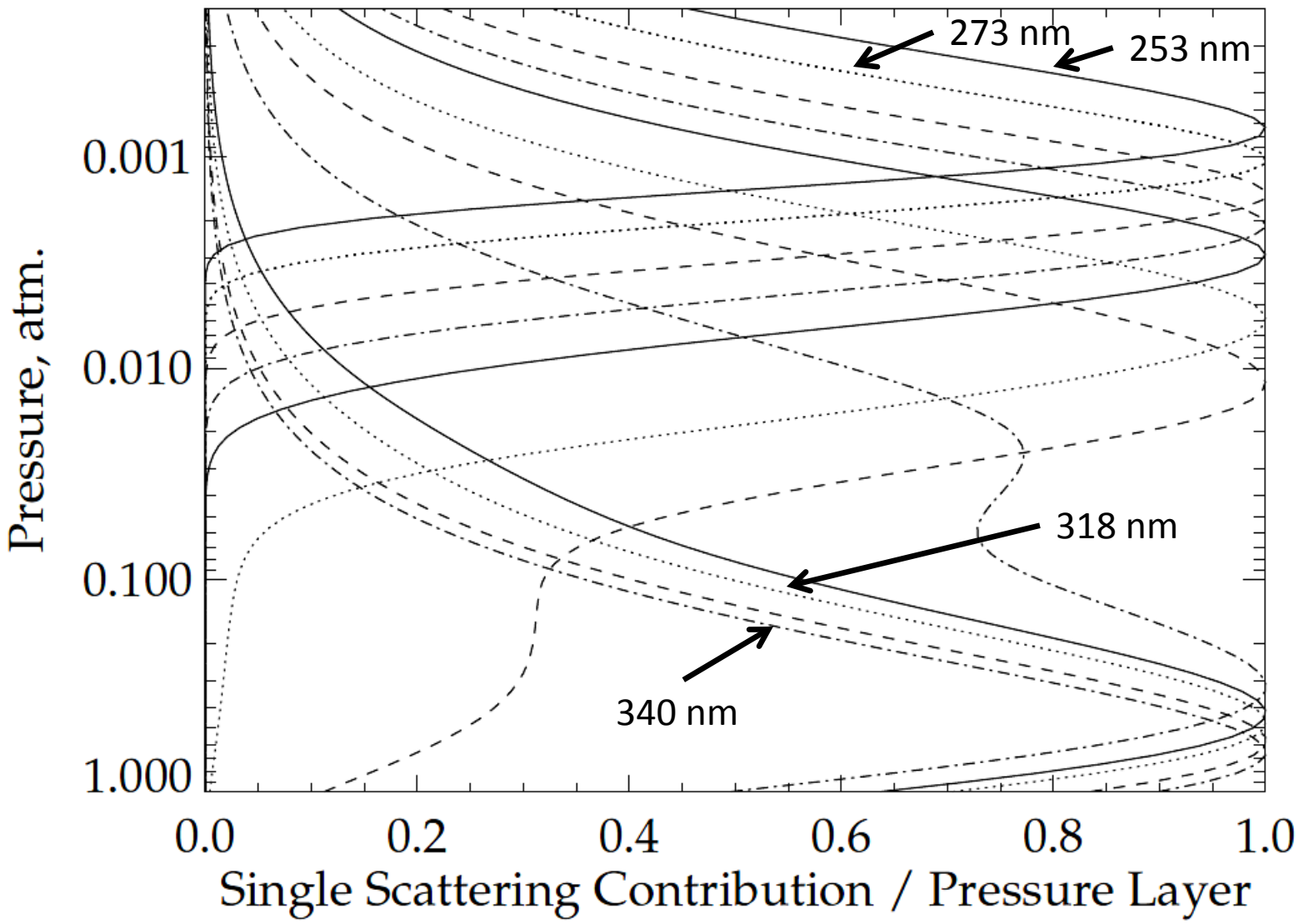
Notes: 1. SDRs will go to 50x50 km^2 for J-01. 2. The OMPS Nadir Profiler performance is expected to degrade in the area of the South Atlantic Anomaly (SAA) due to the impact of periodic charged particle effects in this region. 3. All OMPS measurements require sunlight, so there is no coverage in polar night areas.

Verification of Performance:

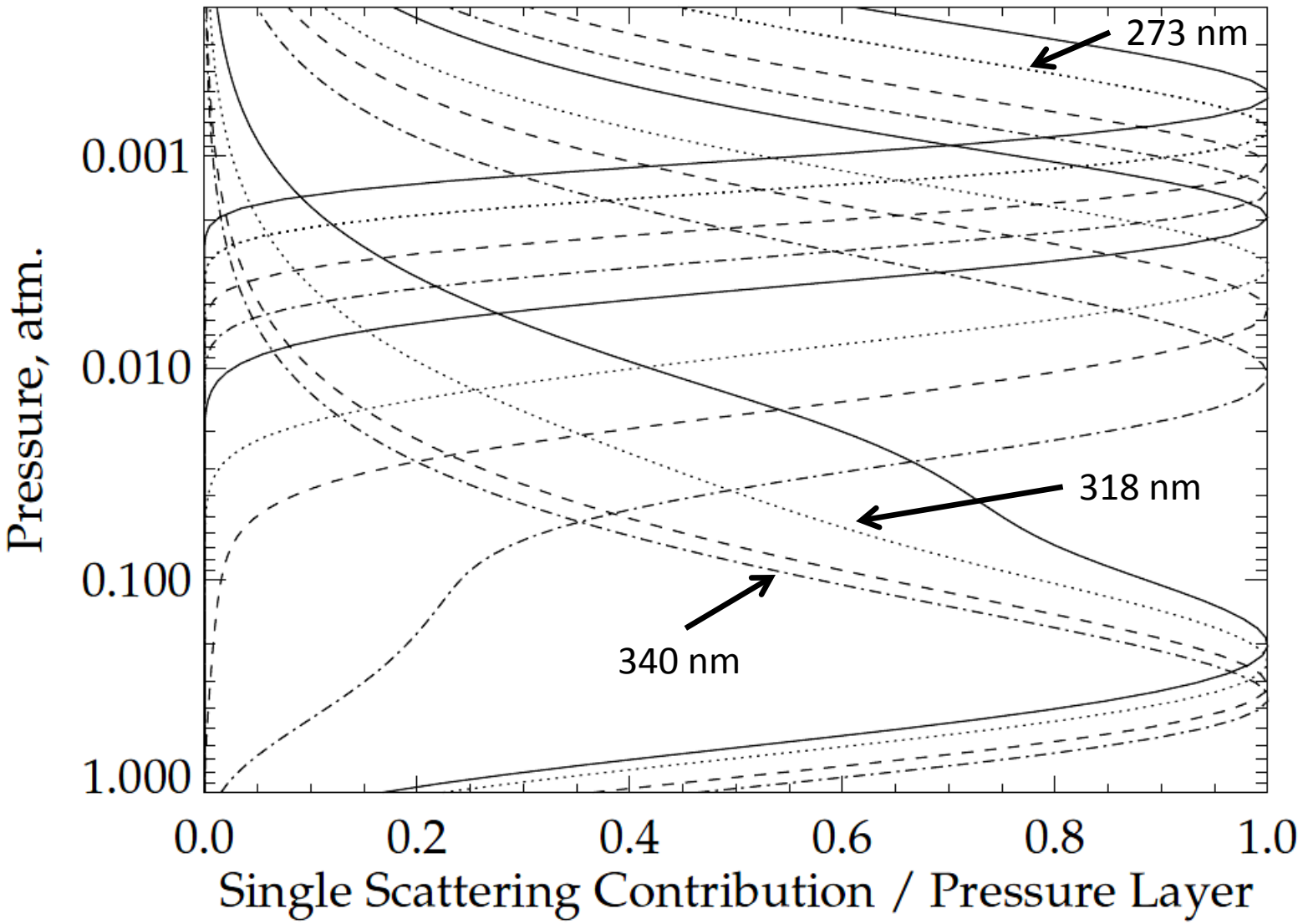
a. 93-Pixel cross-track aggregation and 37.5-S along track integration.
b. Version 8 Algorithms Averaging Kernels
c. Confirmed by to Nadir Mapper, Pixel size, and co-alignment.
d. Confirmed by four years of processing and ground-based matchup scatter.
e. Precision estimates from SNR and Version 8 measurement contribution functions, and along-track differences
f. Accuracy is adjusted by soft calibration and checked by zonal mean statistics, chasing orbits, and Version 8 a priori profiles
g. Suborbital track and precession of orbits.



b. OMPS V8Pro Averaging Kernels for selected layers for two retrievals on December 20, 2015: (a) and (b) are for a retrieval at 49°S, 143°E, with 45° SZA, *R*=0.22 and 294 DU total column ozone; (c) and (d) are for a retrieval at 48°N, 170°E, with 75° SZA, *R*=0.76 and 325 DU total column ozone. The Diamond symbols show the altitudes of the perturbed layers.

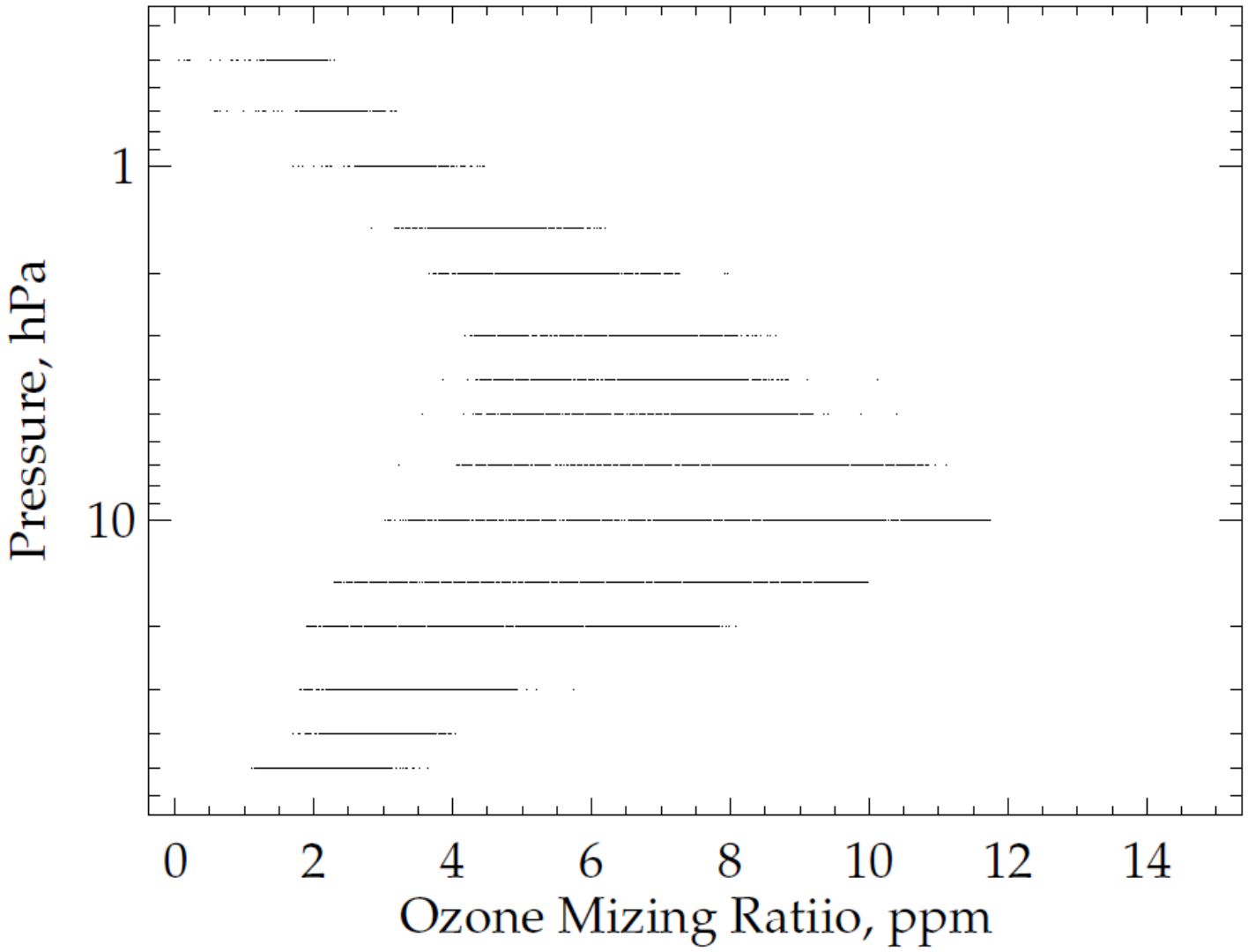


d. Normalized Single Scattering Contribution Functions for 12 wavelengths at [253,273,283,288,292,297,302,306,313,318,331,340] nm for a 325 DU total column ozone profile for Solar Zenith Angle θ_0 = 30°.



d. Normalized Single Scattering Contribution Functions for 12 wavelengths at [253,273,283,288,292,297,302,306,313,318,331,340] nm for a 325 DU total column ozone profile for Solar Zenith Angle θ_0 = 70°.

d. Mixing Ratios for August 25, 2015



d. Measurement range of mixing ratios versus pressure for one day including SAA.

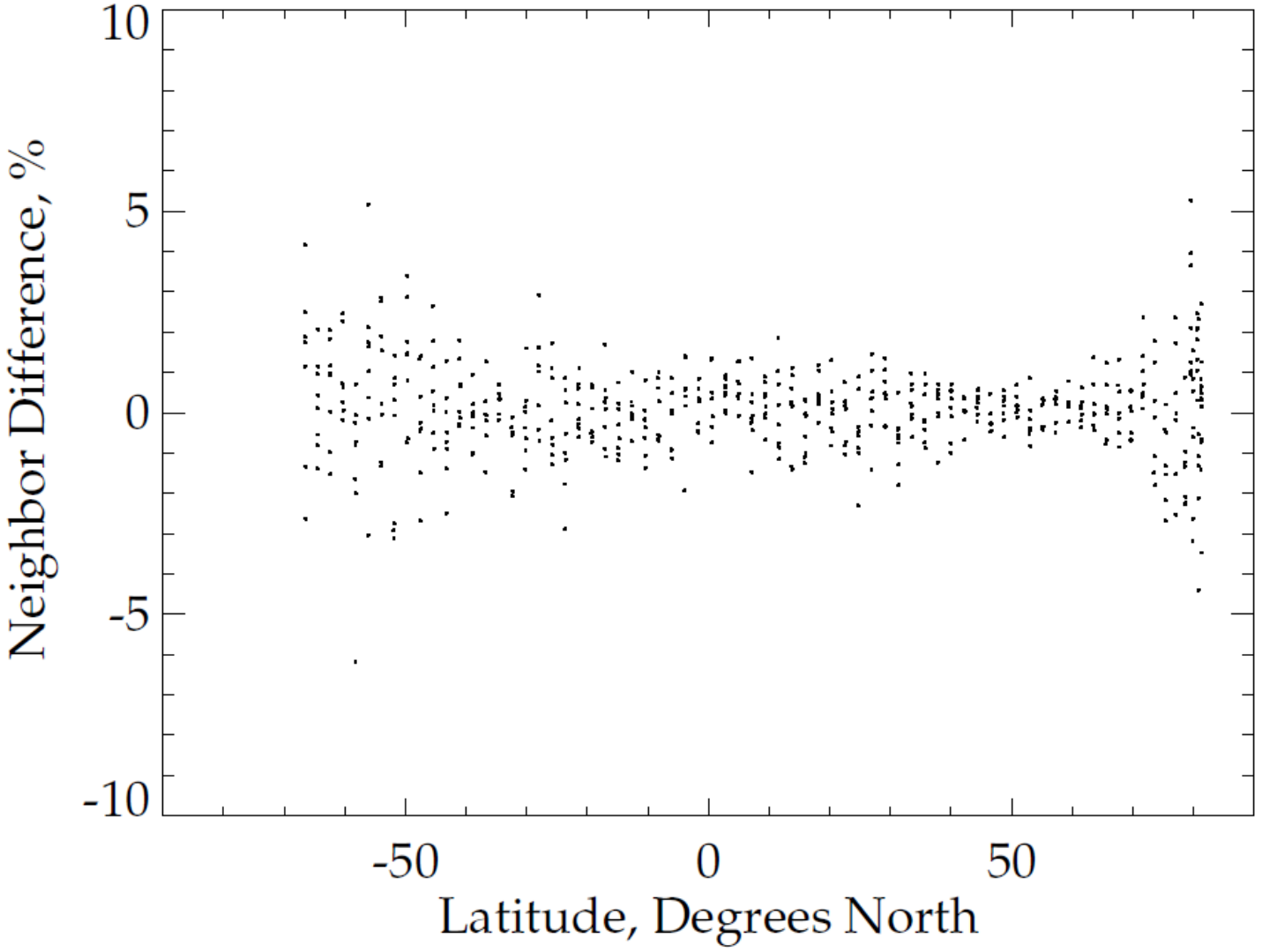
e. SDR Error Impacts on Precision/Accuracy

The sensitivity of the ozone retrievals to radiance/irradiance ratio errors is approximately 1.6%::1%

- Wavelength scale produces radiance variations of ±1%
  - 1.6%/1% x 1% = 1.6% O3 effects

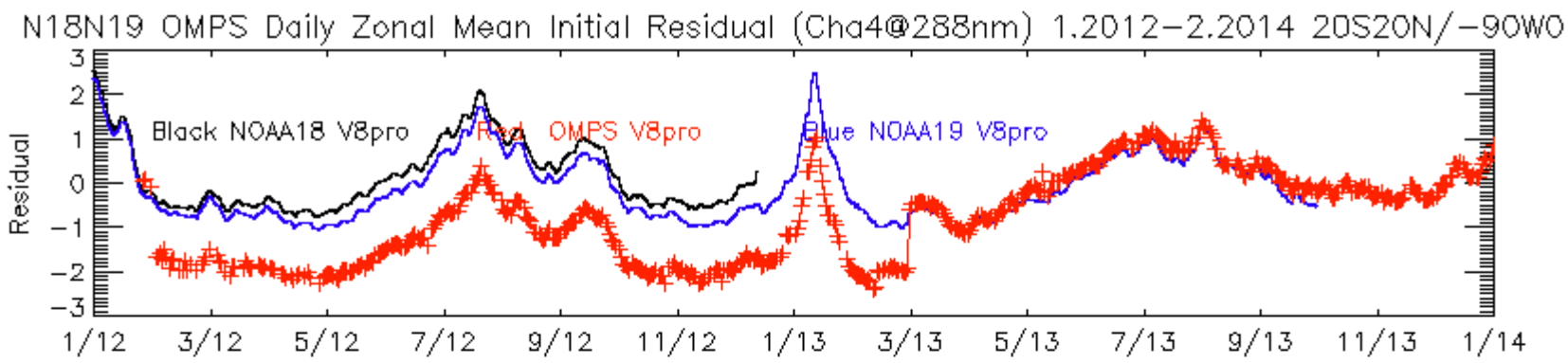
  and ozone cross-section, alpha, of ±0.4 %,
  - 0.02 nm x 100%/5 nm x 1%/1% = 0.4% O3 effects
- Solar activity produces irradiance variations of ±1%
  - 1.6%/1% x 1% = 1.6% O3 effects
- Instrument degradation is -0.5%/year at 253 nm
  - 1.6%/1% x 0.5%/year = 0.8%/year O3 effects (annual update to CFE)
- Stray light errors are now approximately 1/3 of the original errors with radiance variations of ±1%
  - 1.6%/1% x 1% = 1.6% O3 effects

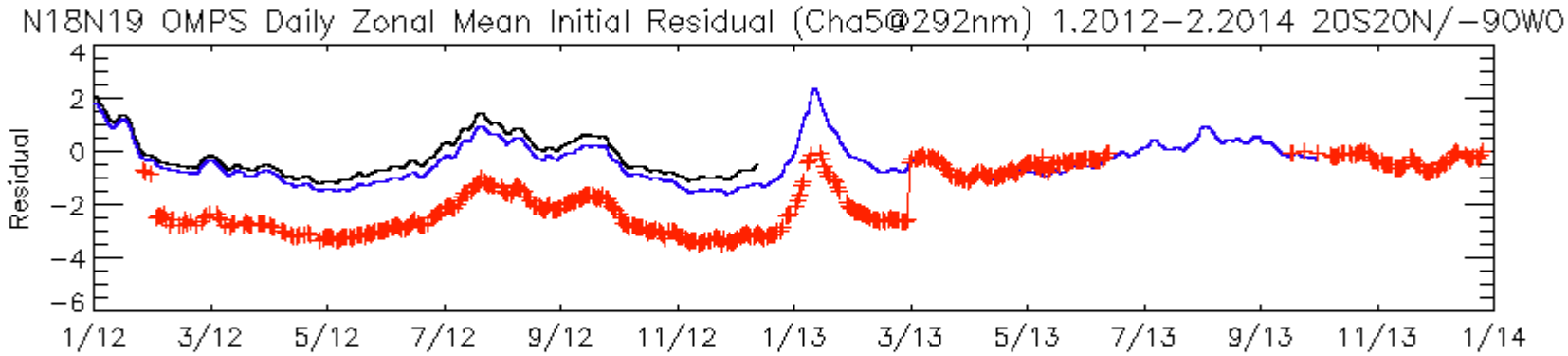
e. Along-Track Differences for August 25, 2015

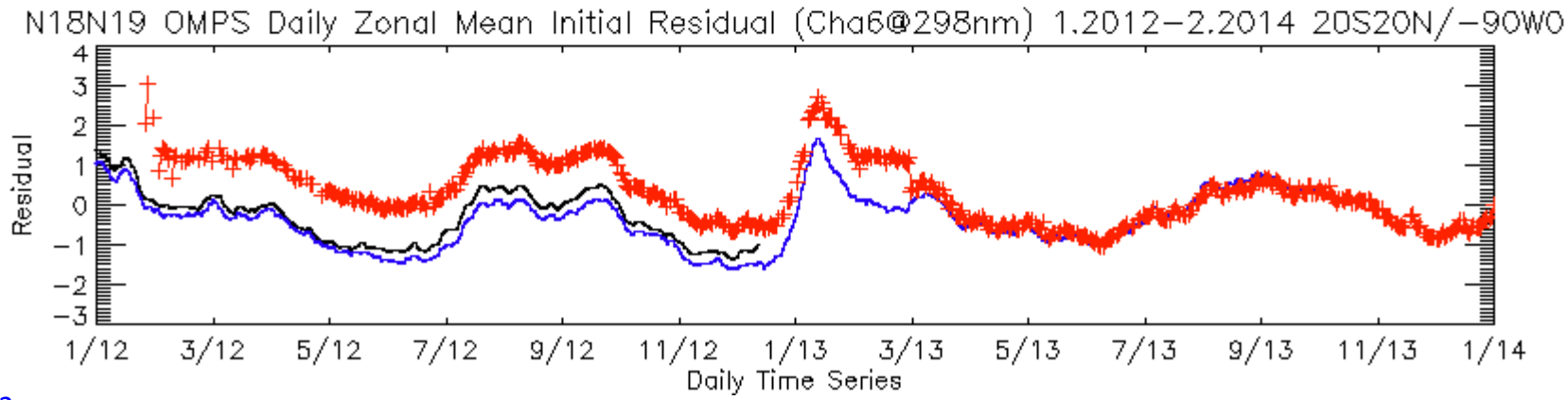


e. Layer ozone difference with averages of adjacent retrievals for Layer 11 of 21 for August 25, 2016. Daily RMS values for layers 2 to 20 are 5.0, 5.5, 5.9, 5.8, 5. 3, 4.3, 2.6, 2.8, 3.2, 2.3, 1.3, 1.2, 1.4, 1.2, 0.9, 1.3, 1.5, 1.5, 1.3 %

f. Initial Residual Biases before/after adjustments







Adjustments using A, K, and Dy

The Averaging Kernel, A, is the product of the Jacobian of partial derivatives of the measurements with respect to the ozone profile layers, K, and the measurement retrieval contribution function, Dy:

$$A = Dy \# K$$

For a linear problem, the retrieved profile, Xr, is the sum of the A Priori Profile, Xa, plus the product of the Averaging Kernel, A, times the difference between the Truth Profile, Xt, and Xa:

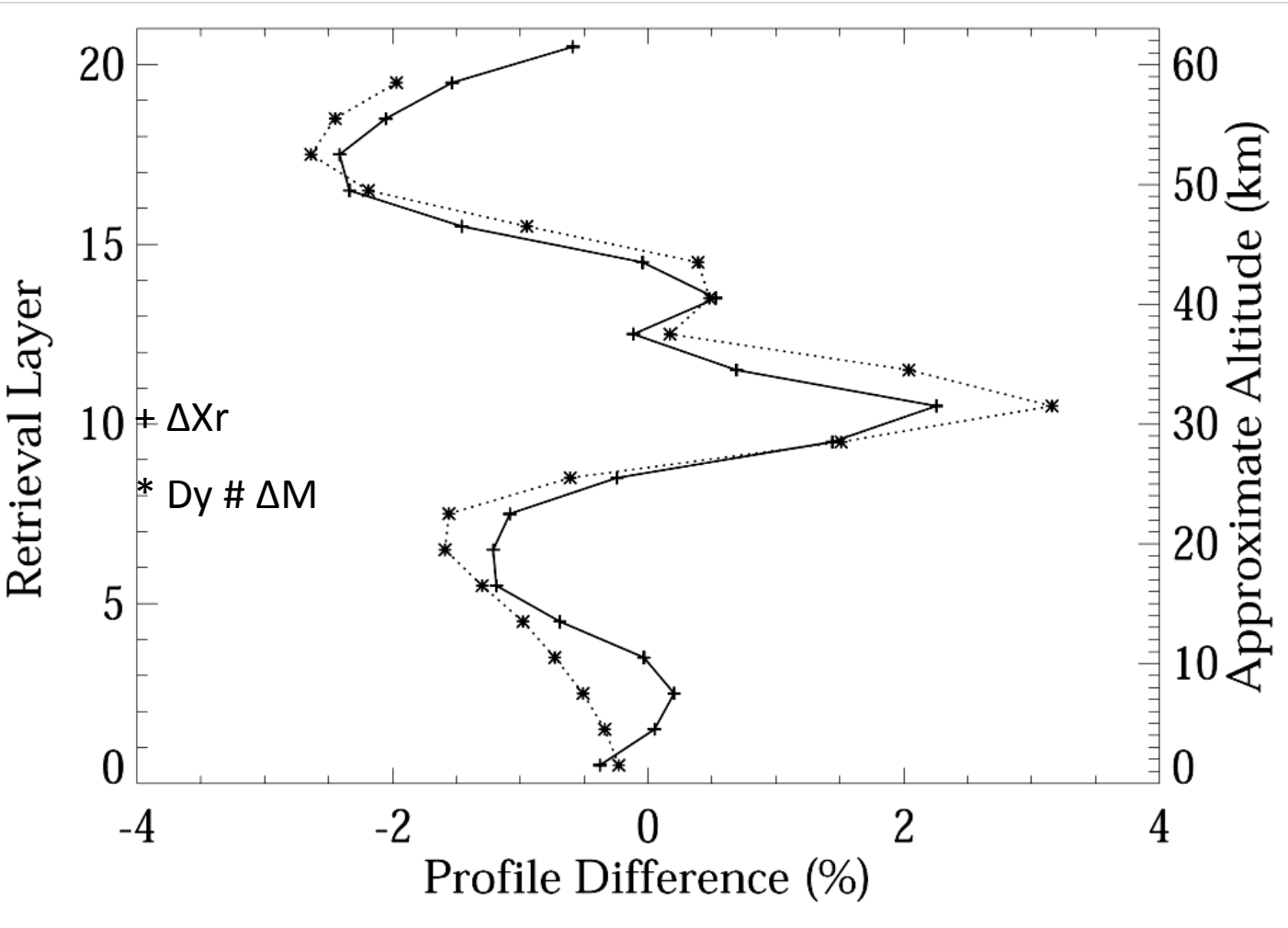
$$Xr = Xa + A \# [Xt - Xa]$$

The measurement change, ΔM, is the Jacobian times a profile change, ΔX:

$$\Delta M = K \# \Delta X$$

The retrieval change, ΔXr, is the contribution function times a measurement change, ΔM:

$$\Delta Xr = Dy \# \Delta M$$



Comparison of actual differences in annual tropical zonal mean profiles retrieved by NOAA-16 and NOAA-17 SBUV/2 for 2003 with those predicted by their differences in their initial residuals. The "+" symbols are Δ**Xr** computed directly from the ozone retrievals and the * symbols are **Dy** Δ**M** with Δ**M** computed from the initial residuals. We can produce vary homogeneous Climate Data Records by determining the Δ**M** values.

f. Chasing Orbit Comparisons to SBUV/2

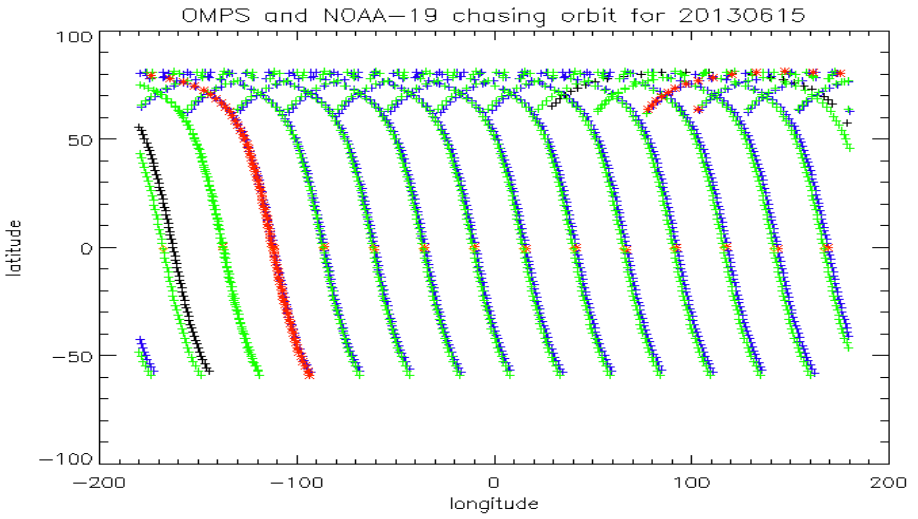
Approximately every 12 days, the orbital tracks for the NOAA-19 and S-NPP spacecrafts align and allow comparisons of products for similar locations with small viewing time differences. The top figure shows convergence of the orbital paths.

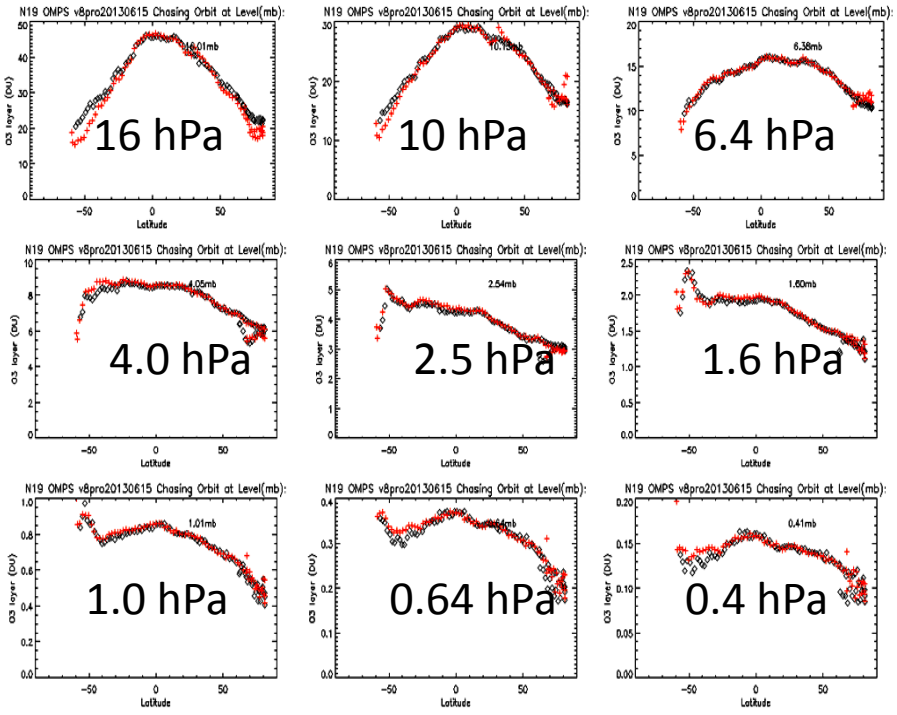
Products and residuals from the same retrieval algorithms for SBUV/2 and OMPS NP can be compared directly. The bottom figures shows ozone amounts for nine layers for the two Version 8 retrievals with the top left for the lowest layer and the bottom right for the highest layer.

Additional monitoring plots provided at

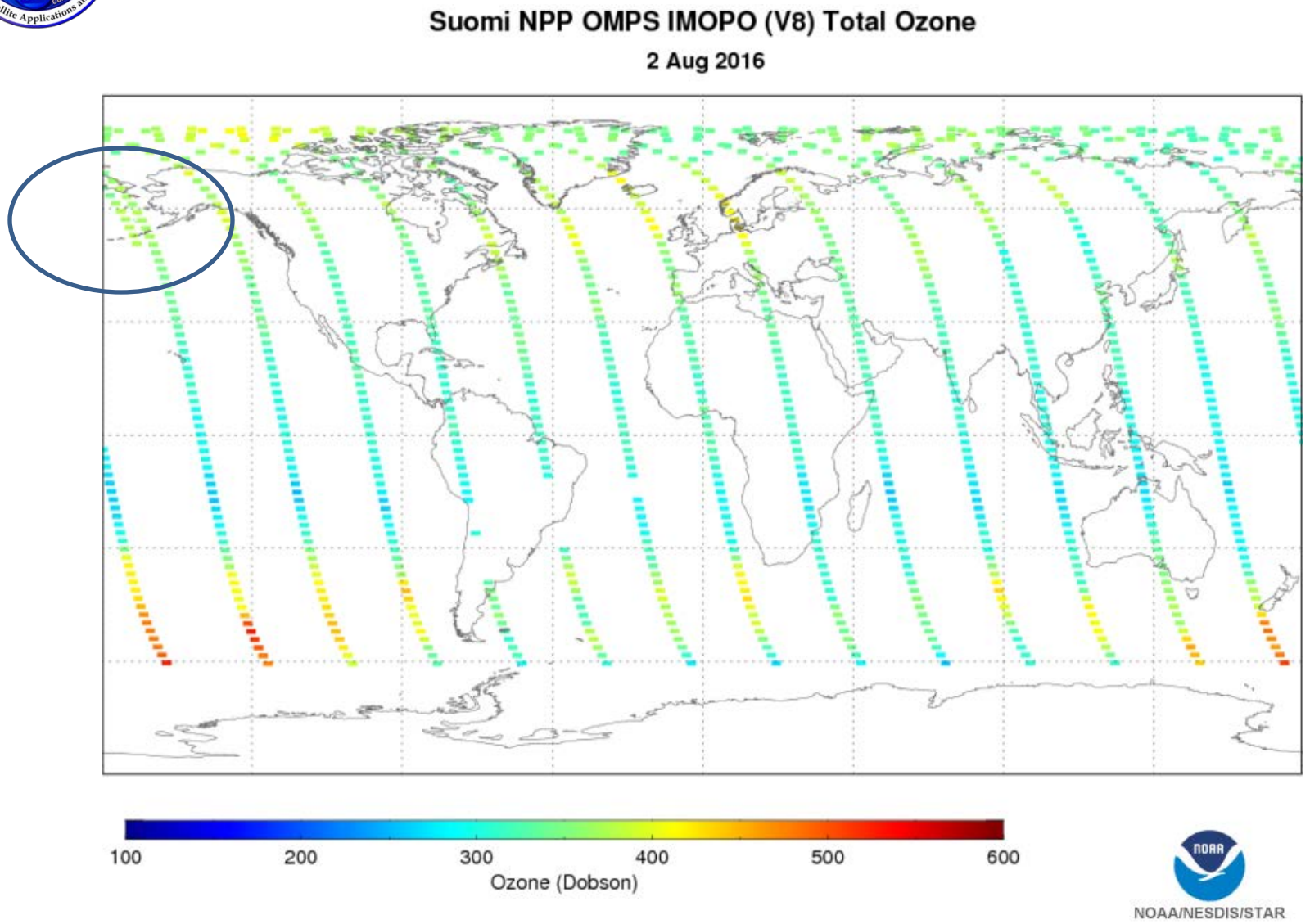
http://www.star.nesdis.noaa.gov/icvs/prodDemos/proOMPSbeta.O3PRO_V8.php

show that the ozone profile differences are consistent with the initial measurement residuals computed relative to the first guess profiles.





Daily Coverage for Nadir Ozone Profile



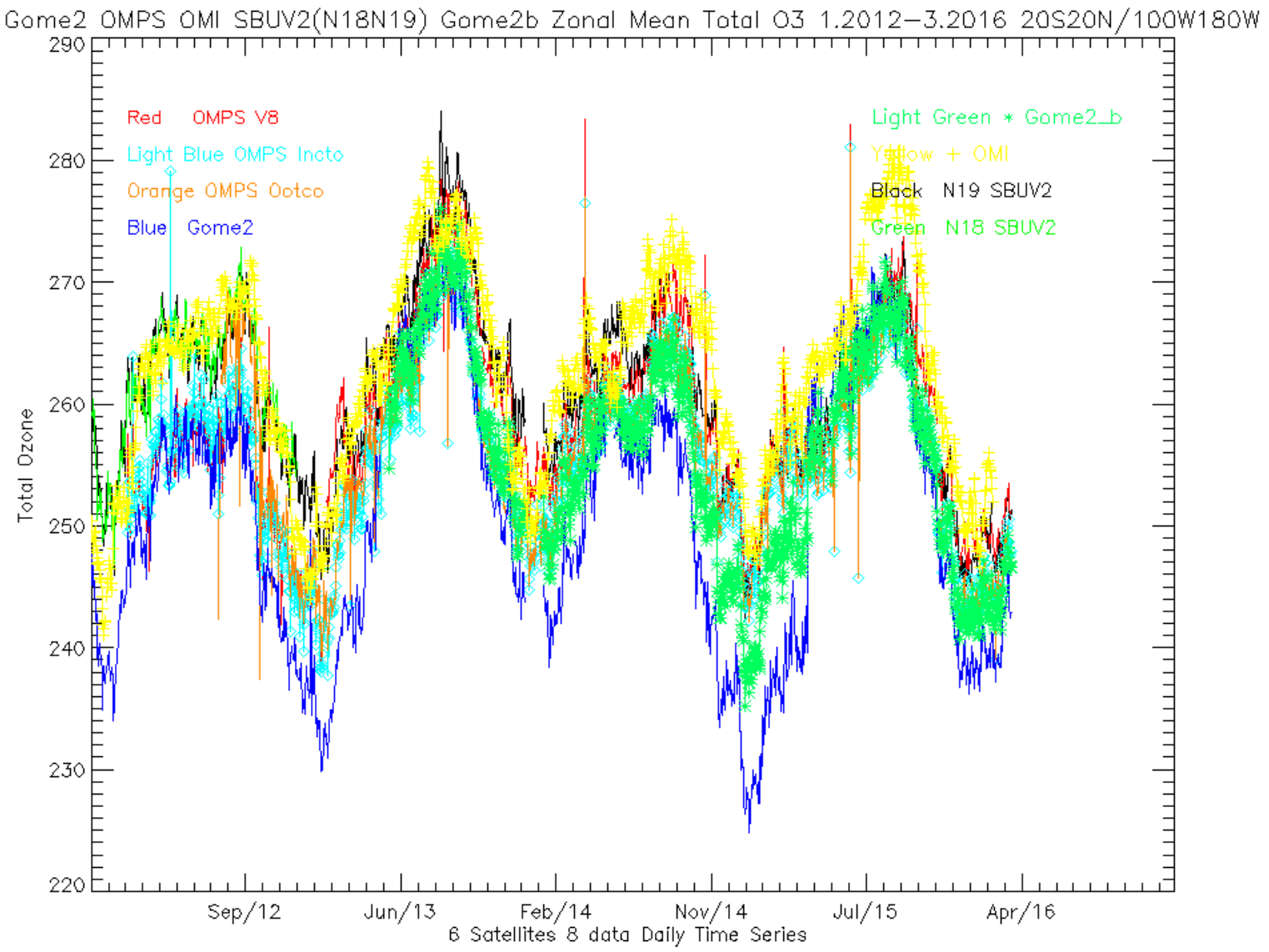
g. Daily coverage of OMPS Nadir Ozone Profile EDR. Note the precession of the orbits in the upper left corner.

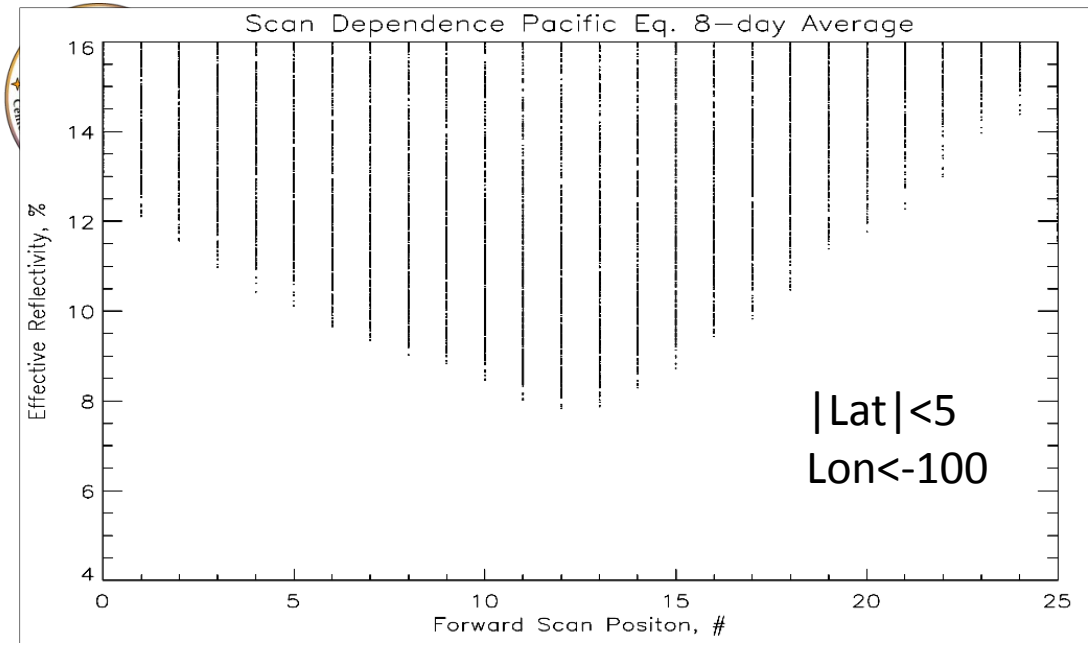
V8 Nadir Ozone Profile Summary

- The heritage, enterprise Version 8 Ozone Profile algorithm is ready for implementation at NDE as part of the redirected EDR processing for JPSS.
- The EDRs from the algorithm meet the required performance levels for the Nadir Ozone Profiles when applied to the validated OMPS NP and NM SDRs.

Backup

(f) Comparisons to other Satellites





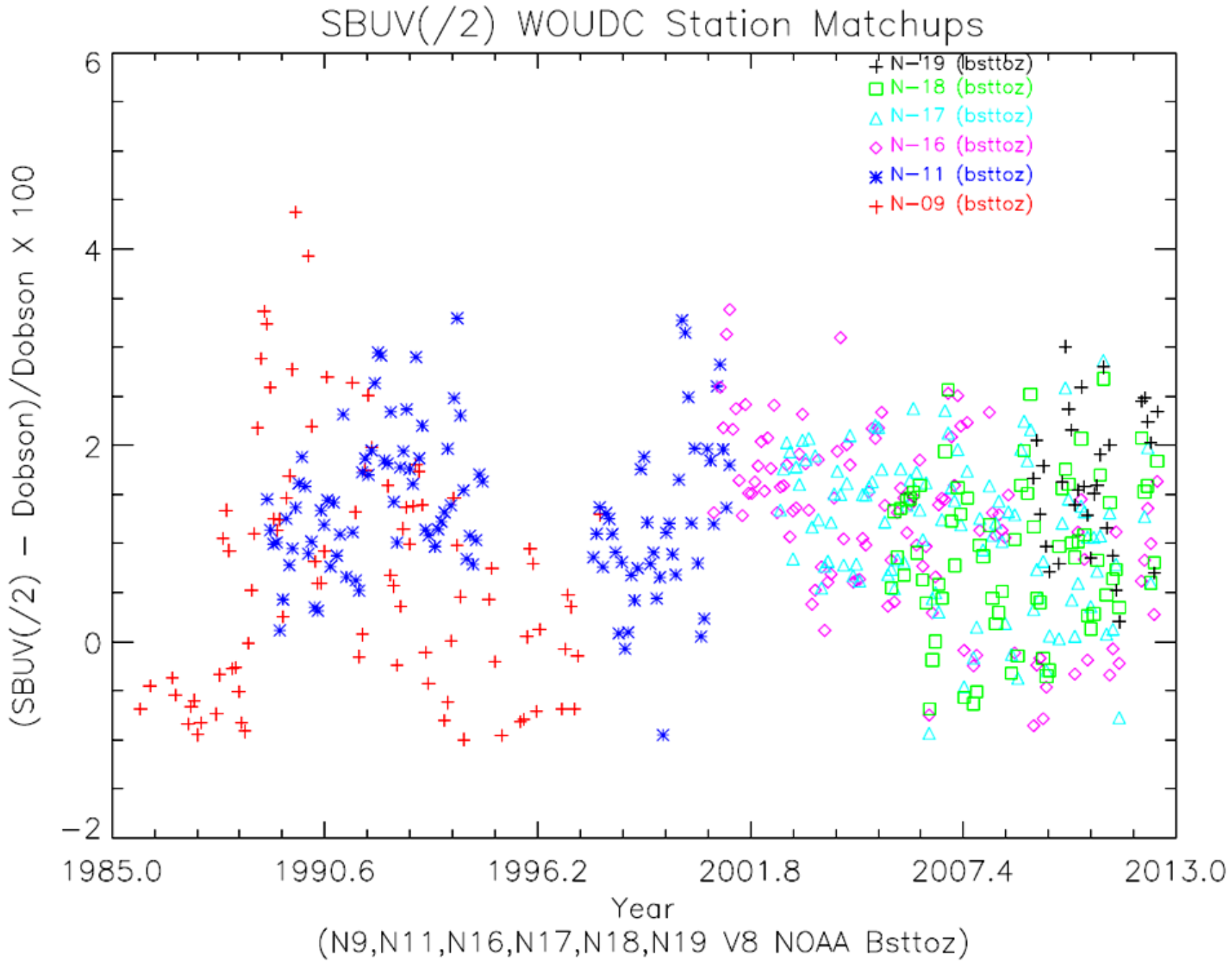
EAST

WEST

Metop-A GOME-2 Version 8 331-nm Reflectivity for a box in the Equatorial Pacific.

The unadjusted values in the top plot reach a minimum of 8% (higher than expected for the open ocean) for the Nadir scan position.

A single calibration adjustment to the 331-nm channel lowers this value to 4% and also flattens out the scan dependence for West-viewing positions. The East-viewing results are not as good but there is sun glint contamination for those angles.


SBUV(/2) WOUDC Station Matchups
N-19 (bsttoz)
N-18 (bsttoz)
N-17 (bsttoz)
N-16 (bsttoz)
N-11 (bsttoz)
N-09 (bsttoz)
(SBUV(/2) - Dobson)/Dobson X 100
6
4
2
0
-2
1985.0
1990.6
1996.2
2001.8
2007.4
2013.0
Year
(N9,N11,N16,N17,N18,N19 V8 NOAA Bsttoz)