Status of Ozone Products

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with contributions from members of the
NOAA JPSS OMPS Ozone Products Team
and
NASA S-NPP OMPS Science Team

May 12, 2014
NOAA STAR JPSS Science Meeting

Outline

- Requirements,
- Team Members
- Instruments/ Measurements
- Products (performance)
- Algorithms
  - Descriptions
  - Recommendations / Paths Forward
- Validation and Applications
- Challenges

Table 2.1.3 - Ozone Total Column		
EDR Attribute	**Threshold (1,2)**	**Objective**
a. Horizontal Cell Size	50 x 50 km^2 @ nadir (10)	10 x 10 km^2 (10)
b. Vertical Cell Size	0 - 60 km	0 - 60 km
c. Mapping Uncertainty, 1 Sigma (3)	5 km at Nadir (3)	5 km
d. Measurement Range	50 - 650 milli-atm-cm	50-650 milli-atm-cm
e. Measurement Precision (4)		
1. X < 0.25 atm-cm	6.0 milli-atm-cm (4,5)	1.0 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	7.7 milli-atm-cm (4,5) ~ 2%	1.0 milli-atm-cm
3. X > 0.45 atm-cm	2.8 milli-atm-cm + 1.1% (4,5)	1.0 milli-atm-cm
f. Measurement Accuracy (6)		
1. X < 0.25 atm-cm	9.5 milli-atm-cm (6,5)	5.0 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	13.0 milli-atm-cm (6,5) ~ 3%	5.0 milli-atm-cm
3. X > 0.45 atm-cm	16.0 milli-atm-cm (6,5)	5.0 milli-atm-cm
g. Latency	120 min. (7)	15 min
h. Refresh	At least 90% coverage of the globe every 24 hours (monthly average) (8)	24 hrs. (8)
i. Long-term Stability (9)	1% over 7 years	0.5% over 7 years
		v1.4.2, 7/29/11

Notes:

1. The OMPS Limb Profiler instrument does not fly on JPSS-1. Thus, only the Ozone Total Column elements are shown in this Table.
2. The loss of the OMPS Limb Profiler has had a small effect on the total column performance as the estimates of the profile shape and the tropospheric ozone are poorer, so the corrections are also poorer. There is new information that the OMPS algorithm use of the IR cloud top pressures will lead to errors as the IR values tend to be higher than the UV ones that should be used. A Discrepancy Report has

Table 4.2.4 - Ozone Nadir Profile (OMPS-NP)		
Attribute	**Threshold**	**Objective**
Ozone NP Applicable Conditions: 1. Clear, daytime only (3)		
a. Horizontal Cell Size	250 X 250 km (1)	50 x 50 km2
b. Vertical Cell Size	5 km reporting	
1. Below 30 hPa (~ < 25 km)	10 -20 km	3 km (0 -Th)
2. 30 -1 hPa (~ 25 -50 km)	7 -10 km	1 km (TH -25 km)
3. Above 1 hPa (~ > 50 km)	10 -20 km	3 km (25 -60 km)
c. Mapping Uncertainty, 1 Sigma	< 25 km	5 km
d. Measurement Range		
Nadir Profile, 0 - 60 km	0.1-15 ppmv	0.01 -3 ppmv (0-TH) 0.1-15 ppmv (TH-60 km)
e. Measurement Precision (2)		
1. Below 30 hPa (~ < 25 km)	Greater of 20 % or 0.1 ppmv	10% (0 -TH)
2. At 30 hPa (~ 25 km)	Greater of 10 % or 0.1 ppmv	3%
3. 30 -1 hPa (~ 25 -50 km)	5% -10%	1%
4. Above 1 hPa (~ > 50 km)	Greater of 10% or 0.1 ppmv	3%
f. Measurement Accuracy (2)		
1. Below 30 hPa (~ < 25 km)	Greater of 10 % or 0.1 ppmv	10% (0 -15 km)
2. 30 -1 hPa (~ 25 -50 km)	5% -10%	5% (15 -60 km)
3. At 1 hPa (~ 50 km)	Greater of 10 % or 0.1 ppmv	5% (15 -60 km)
4. Above 1 hPa (~ > 50 km)	Greater of 10 % or 0.1 ppmv	5% (15 -60 km)
g. Refresh	At least 60% coverage of the globe every 7 days (monthly average) (2,3)	24 hrs. (2,3)
	(16.7° FOV)	v2,0, 9/22/12

Notes: 1. The SBUV/2 has a 180 km X 180 km cross-track by along -track FOV. It makes its 12 measurements over 24 Samples (160 km of along-track motion). The OMPS Nadir Profiler is designed to be operated in a mode that is able to subsample the required HCS. 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.

OMPS LP Performance Requirements

The OMPS Limb Profiler provides global ozone observations at high vertical resolution (< 3 km). This EDR provides a measurement of ozone concentration within a specified volume.

Requirements are TBD per L1RDS V2.9 Action: Insert OMPS Limb Profiler SDR Performance Characteristics – Deferred until S-NPP Ozone Limb Profile performance is sufficiently validated to constrain the JPSS-2 instrument acquisition.

Table 3.3.1 - Ozone Limb Profile

Attribute	Threshold (1)	Objective
a. Horizontal Cell Size	250 km	100 km (7)
b. Vertical Cell Size		
1. 0 to TH (2)	N/A	3 km
2. Th to 25 km	5 km	1 km
3. 25 to 60 km)	5 km	3 km
c. Mapping Uncertainty, 1 Sigma (3)	< 25 km	25 km
d. Measurement Range		
1. 0 to TH (2)	N/A	0.01 to 3 ppmv
2. Th - 60 km	0.1 to 15 ppmv	0.1 to 15 ppmv
e. Measurement Precision		
1. 0 to TH (2)	N/A	10%
2. Th to 15 km	Greater of 10 % or 0.1 ppmv	3%
3. 15 to 50 km	Greater of 3 % or 0.05 ppmv	1%
4. 50 to 60 km	Greater of 10% or 0.1 ppmv	3%
f. Measurement Accuracy		
1. 0 to TH (2)	N/A	10%
2. Th to 15 km	Greater of 20 % or 0.1 ppmv	10%
3. 15 to 60 km	Greater of 10 % or 0.1 ppmv	5%
g. Latency	120 min. (4)	15 min
h. Refresh	At least 75% coverage of the globe every 4 days (monthly average) (5)	24 hrs (5)
i. Long-term Stability (6)	2% over 7 years	1% over 7 years
		v1.4.2, 7/29/11

Notes:

Sulfur Dioxide (SO2) Total Column EDR Description & Requirements Table – CCR in preparation

The Sulfur Dioxide Total Column EDR (also called Atmospheric SO_2) is defined as the amount of SO2 in a vertical column of the atmosphere measured in Dobson Units (milli-atm-cm). SO_2 absorption in the 305 nm to 315 nm region influence OMPS Nadir Mapper measurements of backscattered Ultraviolet radiances. Estimates of atmospheric SO_2 are obtained for three or more assumed heights for the amounts within the column averaged over the FOV from measurement residuals calculated by the OMPS total column ozone EDR algorithm. This product will continue the heritage SO_2 Index provided in the NOAA POES SBUV/2 operational Product Master File and the Atmospheric SO_2 products currently provided in NRT products from the NASA EOS Aura OMI.

Note: J1 will not have an SO_2 performance exclusion, so improved information on amounts and corrections to the ozone product will be required.

OMPS Nadir Mapper Atmospheric SO_2 Column Amount in DU*

	Threshold	Objective
a. Horizontal Cell Size:	25x25 KM^2	10X10 KM^2
b. Vertical Reporting NA	Column amount*	
c. Mapping Uncertainty, 3 Sigma	5 KM	2 KM
d. Measurement Precision	2 DU	0.5 DU
e. Measurement Accuracy	3 DU	1 DU
f. Measurement Uncertainty		
g. Latency	80 Minutes	30 Minutes
h. Refresh		

Daily global sunlit Earth** (multiple coverage at high latitudes)

* SO_2 column amounts will be reported as calculated for three heights as appropriate for their occurrence -- local pollution, transported pollution, volcanic eruption.

** SO_2 is not sensed below clouds

Ozone Cal/Val Team Membership

EDR	Name	Organization	Task
Lead	Lawrence Flynn	NOAA/NESDIS/STAR	Lead Ozone EDR Team
Member	Irina Petropavlovskikh	NOAA/ESRL/CIRES	Ground-based Validation Lead
Member	Craig Long	NOAA/NWS/NCEP	Product Application Lead
Member	Trevor Beck	NOAA/NESDIS/STAR	Algorithm development and ADL implementation
Member	Jianguo Niu	STAR/IMSG/SRG	Algorithm development, trouble shooting, Limb Profiler science
Member	Eric Beach	STAR/IMSG	Validation, ICVS/Monitoring, Data management
Member	Zhihua Zhang	STAR/IMSG	V8 Algorithms implementation & modification
Member	Eve-Marie Devaliere	STAR/ERT	Limb Profiler Research to operations
JAM	Maria Caponi	JPSS/Aerospace	Coordination
Member	Bhaswar Sen	NGAS	Current Algorithms

OMPS Fundamentals

NOAA, through the Joint Polar Satellite System (JPSS) program, in partnership with National Aeronautical Space Administration (NASA), launched the Suomi National Polar-orbiting Partnership (S-NPP) satellite on October 28, 2011. The Ozone Mapping and Profiler Suite (OMPS) consists of two telescopes feeding three detectors measuring solar radiance scattered by the Earth's atmosphere and solar irradiance by using diffusers. The measurements are used to generate estimates of total column ozone and vertical ozone profiles.

The nadir mapper (total column) sensor uses a single grating monochromator and a CCD array detector to make measurements every 0.42 nm from 300 nm to 380 nm with 1.0-nm resolution. It has a 110° cross-track FOV and 0.27° along-track slit width FOV. The measurements are currently combined into 35 cross-track bins: 3.35° (50 km) at nadir, and 2.84° at ±55°. The resolution is 50 km along-track at nadir, with a 7.6-second reporting period. The instrument is capable of making measurements with much better horizontal resolution.

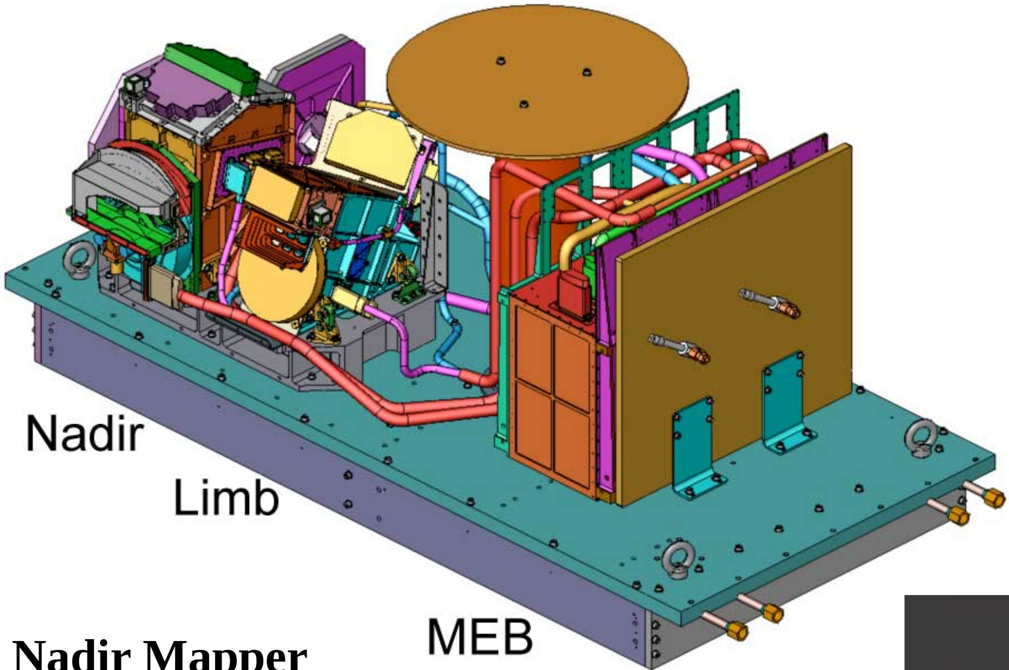
The nadir profiler sensor uses a double monochromator and a CCD array detector to make measurements every 0.42 nm from 250 nm to 310 nm with 1.0-nm resolution. It has a 16.6° cross-track FOV, 0.26° along-track slit width. The current reporting period is 38 seconds giving it a 250 km x 250 km cell size collocated with the five central total column cells.

The limb profiler sensor is a prism spectrometer with spectral coverage from 290 nm to 1000 nm. It has three slits separated by 4.25° with a 19-second reporting period that equates to 125 km along-track motion. The slits have 112 km (1.95°) vertical FOVs equating to 0 to 60 km coverage at the limb, plus offsets for pointing uncertainty, orbital variation, and Earth oblateness. The CCD array detector provides measurements every 1.1 km with 2.1-km vertical resolution. The measurements are used to generate high vertical resolution ozone and aerosol profiles down to the tropopause.

OMPS

Ozone Mapper Profiler Suite

Global daily monitoring of three dimensional distribution of ozone and other atmospheric constituents. Continues the NOAA SBUV/2, EOS-AURA OMI and SOLSE/LORE records.



Nadir Mapper

Grating spectrometer, 2-D CCD
110 deg. cross track, 300 to 380 nm spectral, 1.1nm FWHM bandpass

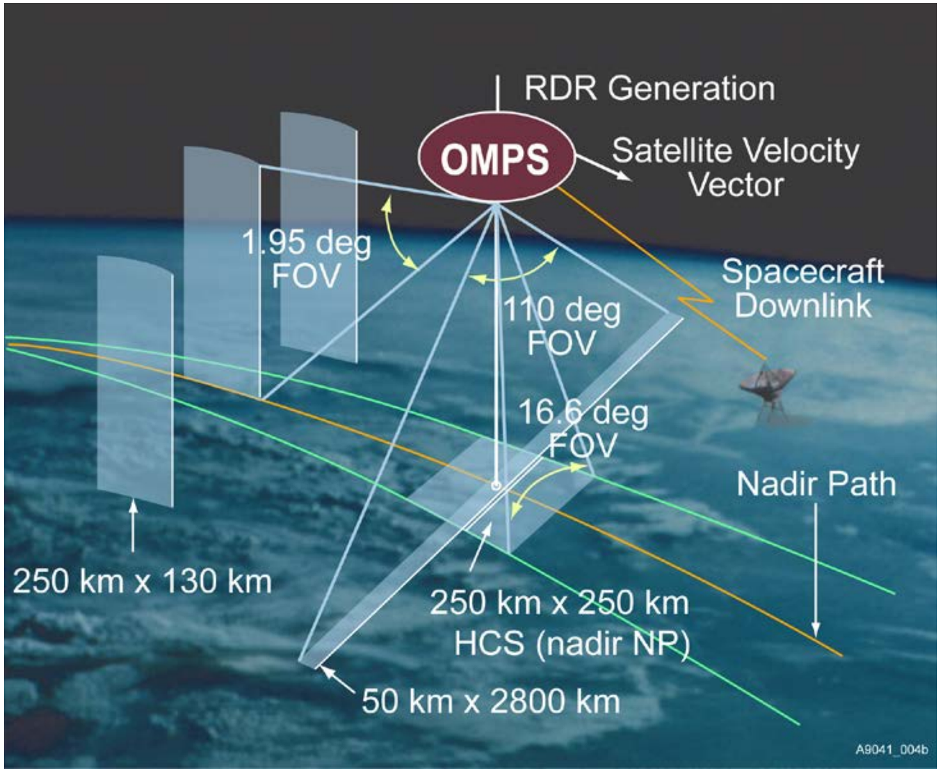
Nadir Profiler

Grating spectrometer, 2-D CCD
Nadir view, 250 km cross track, 270 to 310 nm spectral, 1.1 nm FWHM bandpass

Limb Profiler

Prism spectrometer, 2-D CCD
Three vertical slits, -20 to 80 km vertical, 290 to 1000 nm spectral

The calibration systems use pairs of working and reference solar diffusers.



L. Flynn

Categories of products

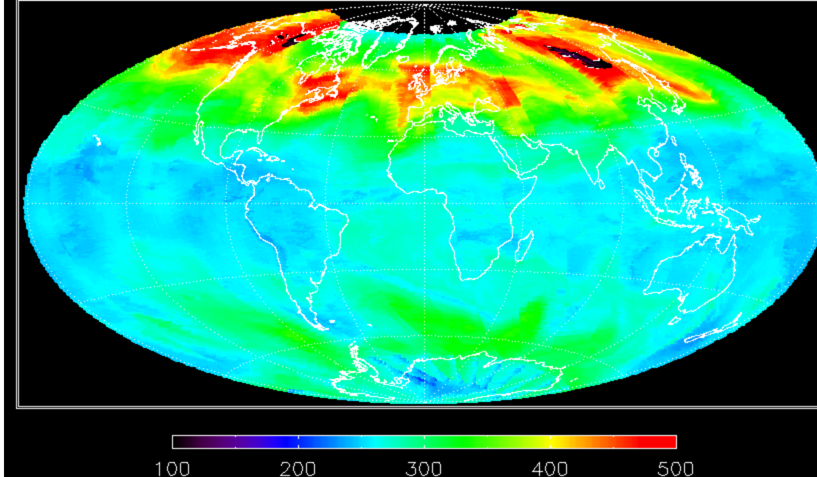
- In operations
  - Total column O_3, Nadir UV O_3 Profile, Aerosol Index, SO_2 Index
  - TOAST combined UV/IR analysis map
  - NUCAPS (CrIS/ATMS) trace gases (O_3, CO, CH_4, CO_2, N_2O, HNO_3, SO_2)
- Planned products
  - Limb O_3 Profile, Limb aerosol profile
- Likely future products
  - Total column SO_2
- Research products
  - Total Column NO_2
  - Combined UV/IR retrieval
  - UV absorbing aerosol optical depth, combined UV/Vis
  - UV cloud optical centroid (inelastic scattering – Ring effect)

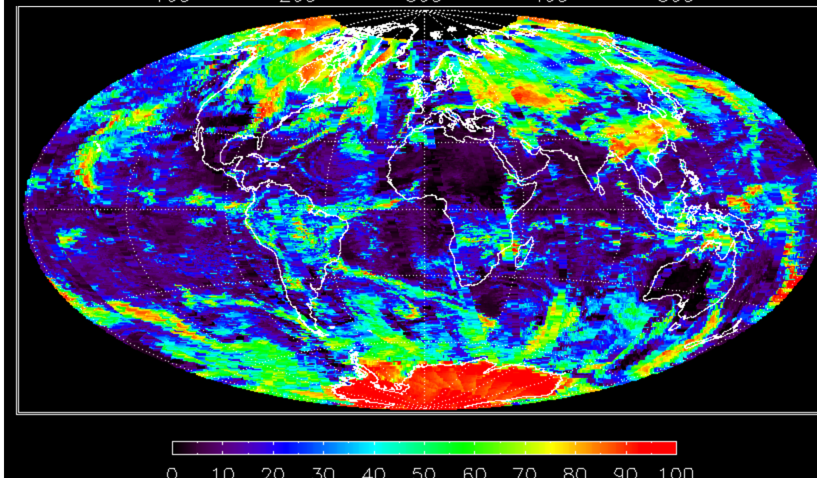
The overall operational retrieval algorithm is working well but there are cross-track calibration biases. These will be corrected by July 2014.

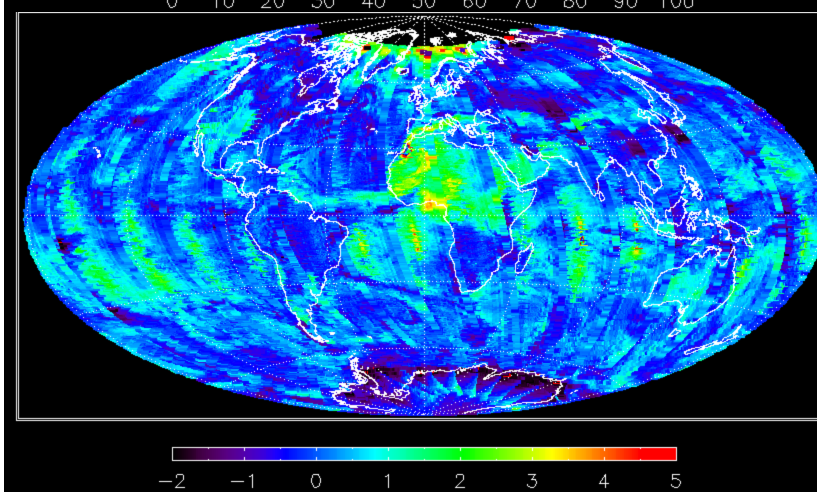
Daily global maps with false color images of three OMPS Version 8 algorithm products for February 17, 2014:
Top – Total column product. The color bar gives the amounts in Dobson Units (1 DU = 1 milli-atm-cm);
Middle – Effective Reflectivity. The colors show varying reflectivity in percent; and
Bottom – Absorbing aerosol index product. The colors show different levels of the index computed as a measurement residual for the 360 nm channel using the reflectivity estimate from the 331 nm channel. The units are in N-values which are approximately equivalent to 2.3% per unit. Sun-glint regions have not been filtered in this map.

Daily images for the full record to date are available through links at

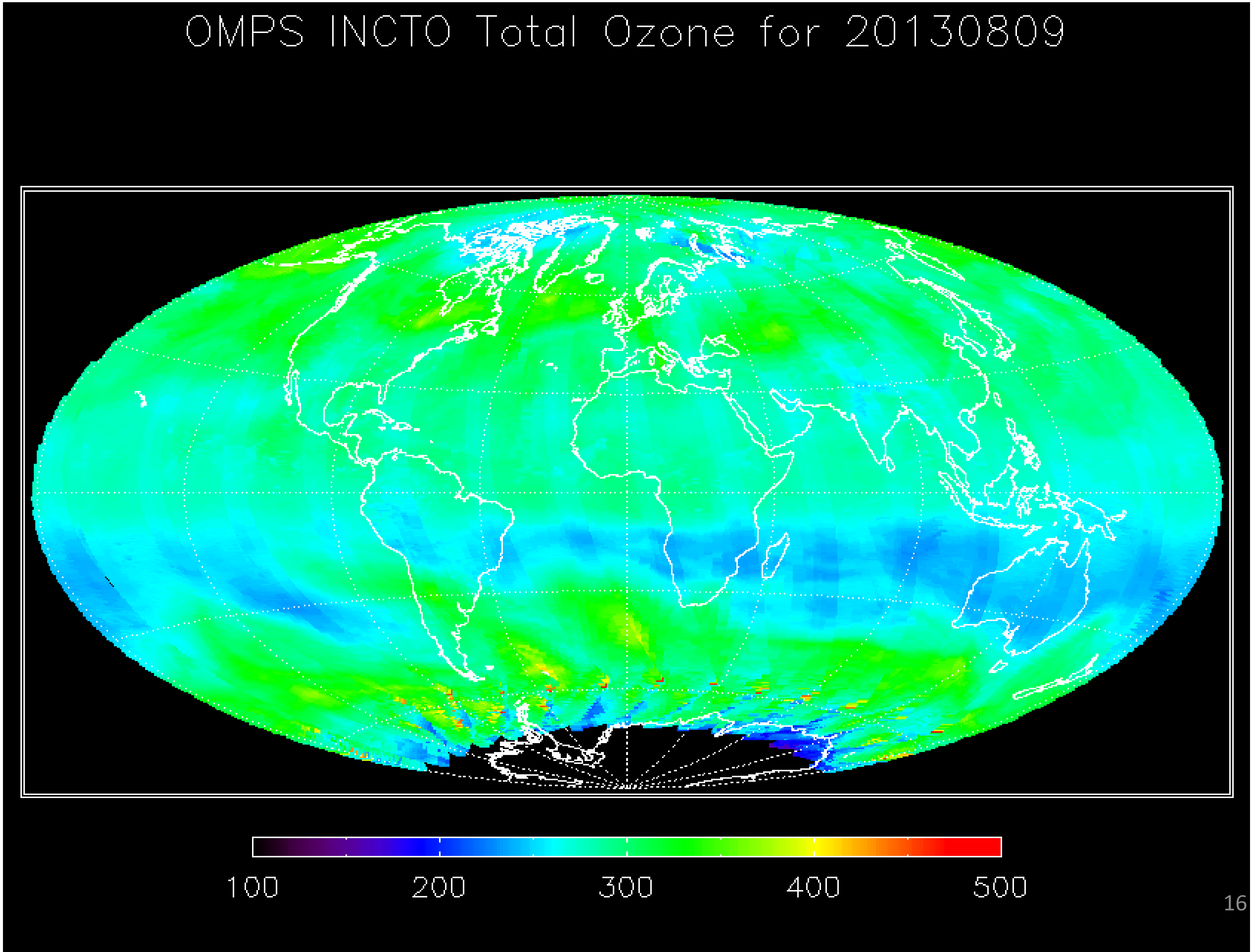
www.star.nesdis.noaa.gov/icvs/index.php.



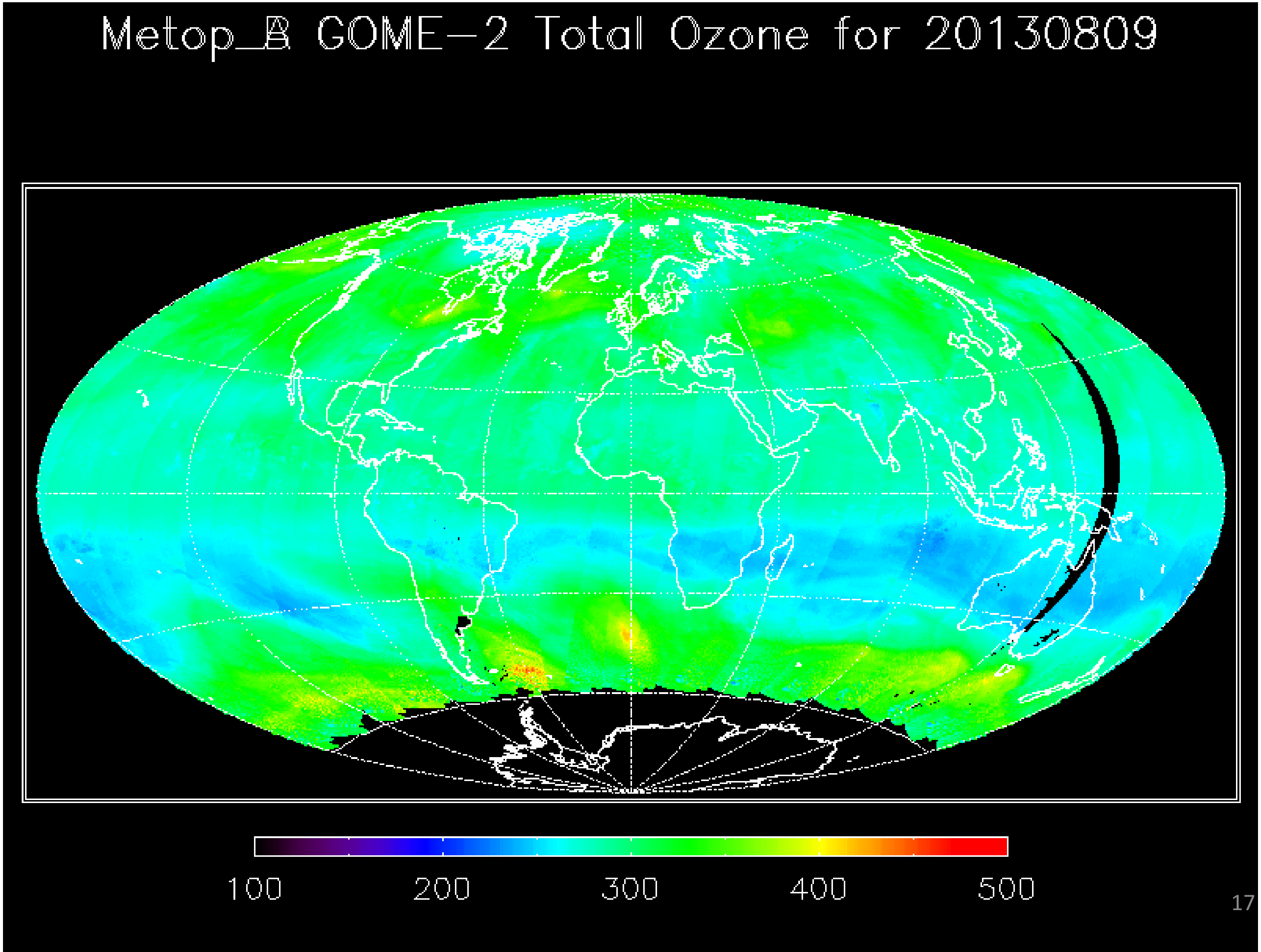




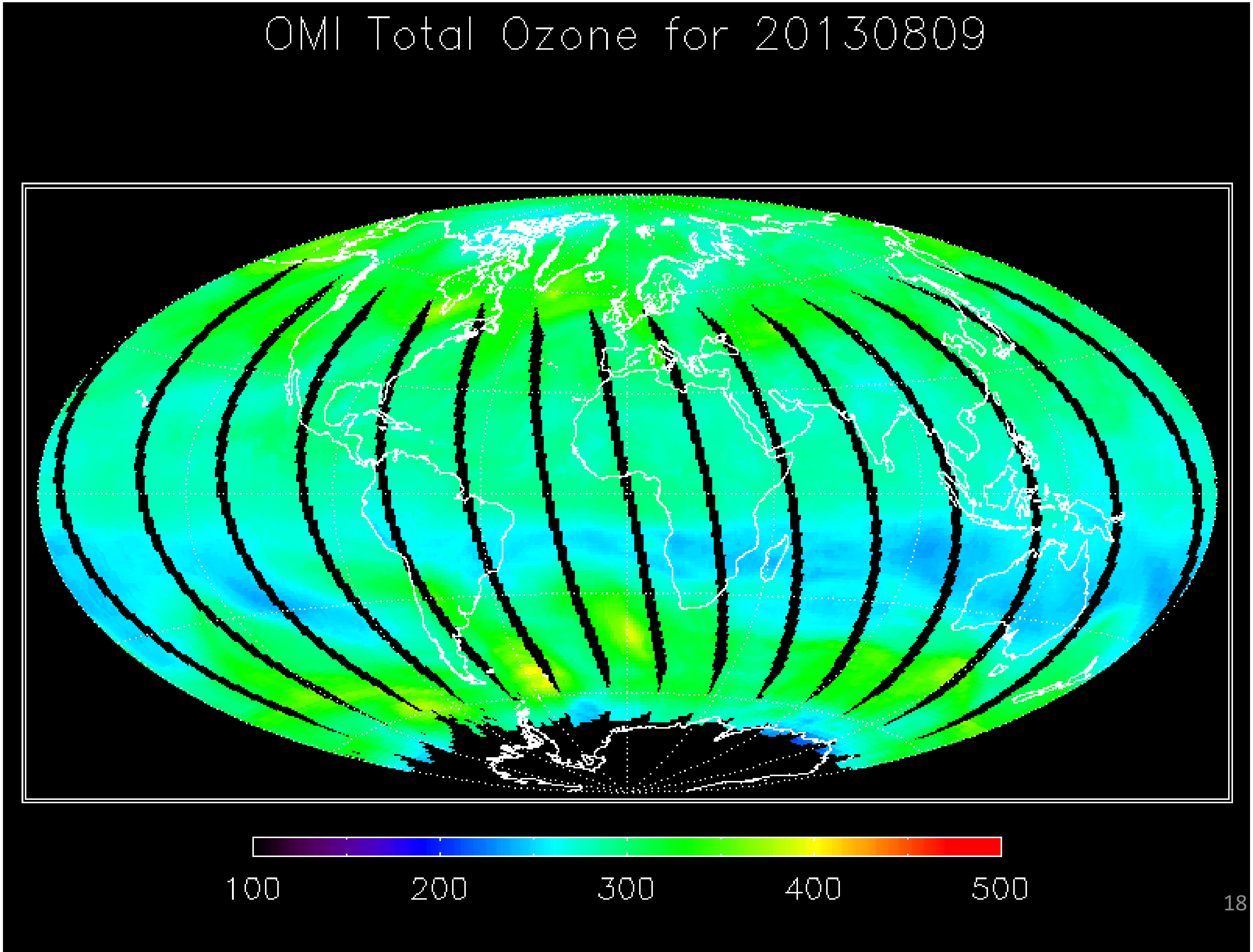
Sample OMPS INCTO Total Ozone Map



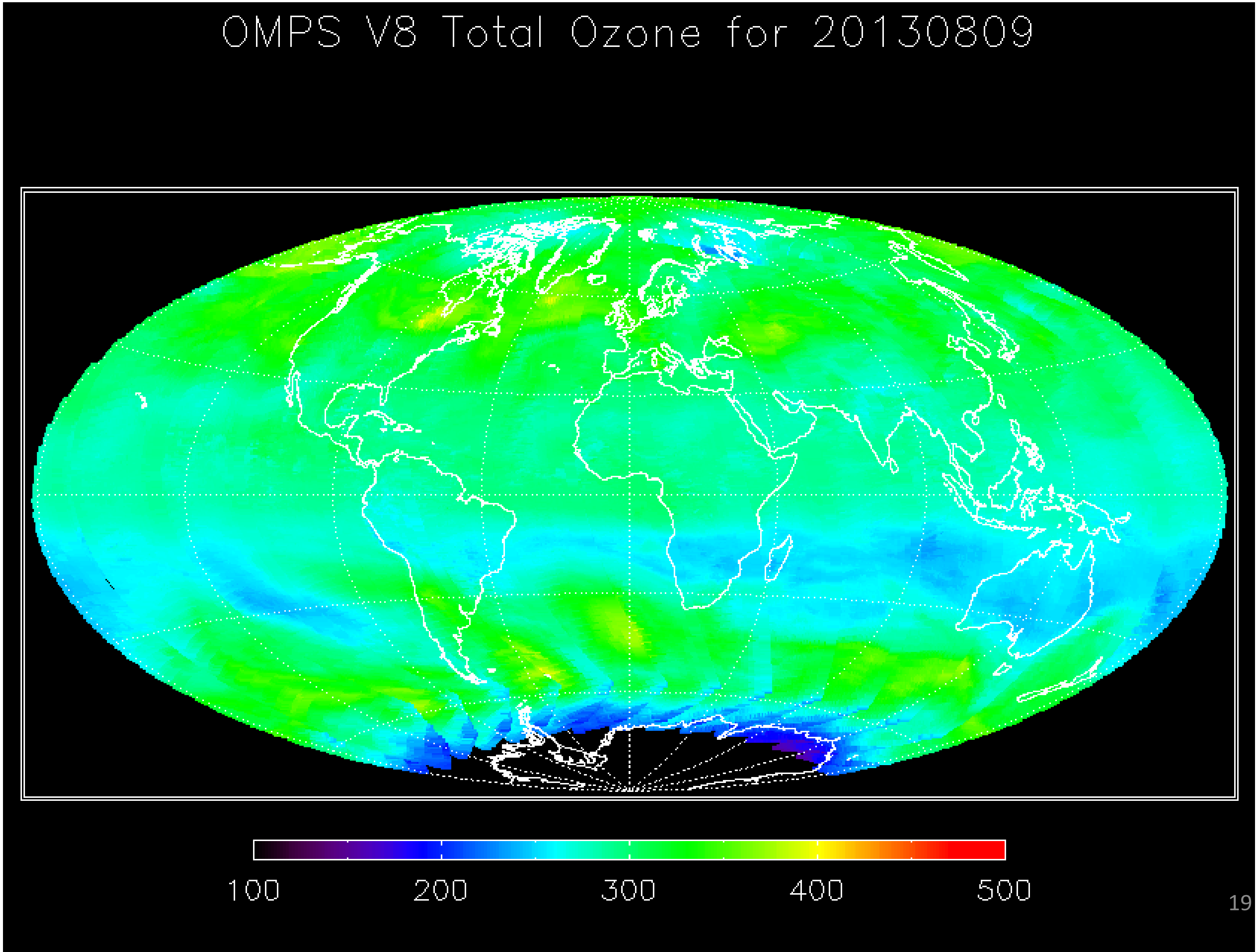
Sample MetOp-A+B GOME-2 V8 Total Ozone Map

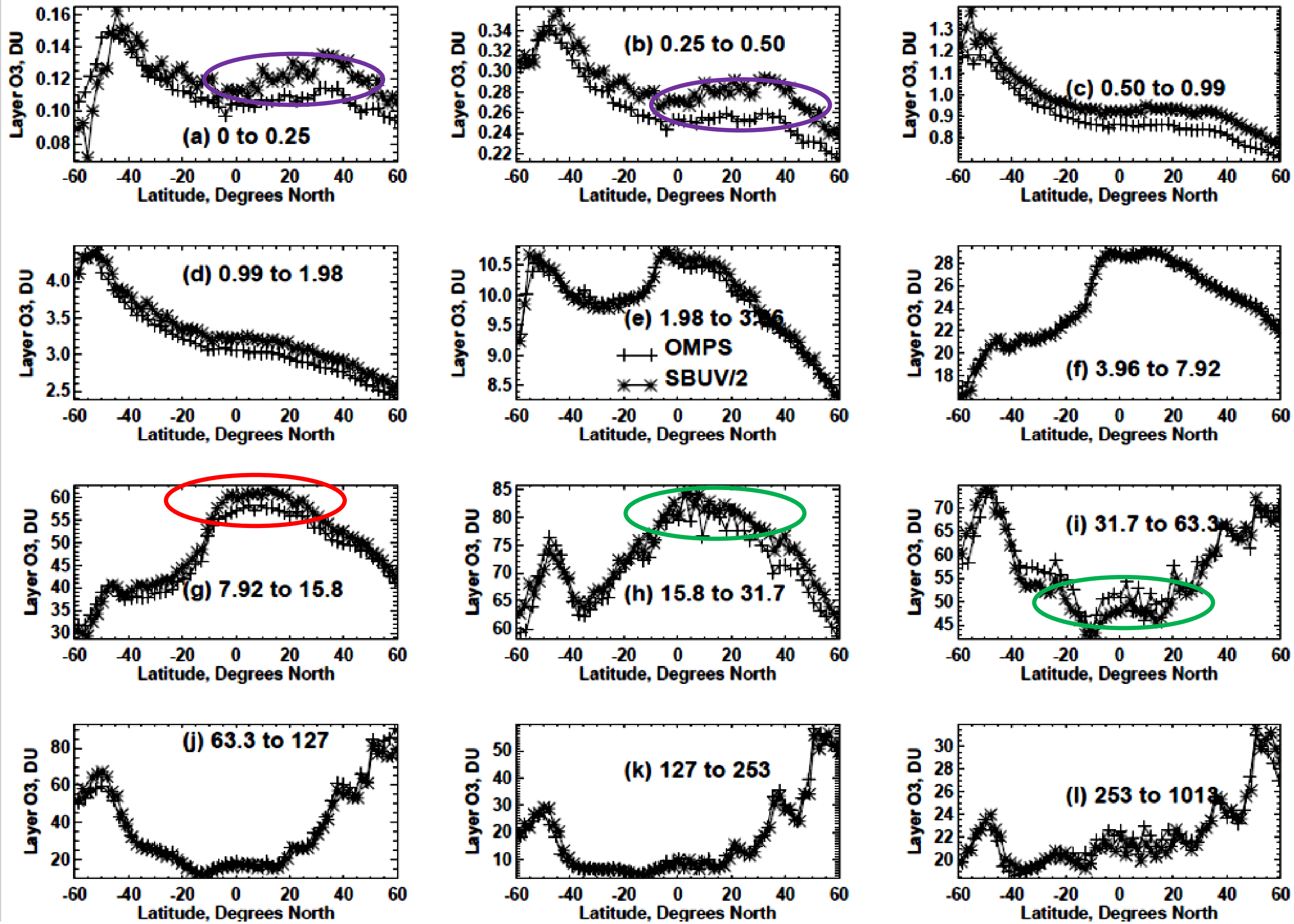


Sample EOS Aura OMI Total Ozone Map



Sample OMPS V8TOZ Total Ozone Map





Biases and offsets from stray light, initial calibration errors and mismatched FOVs appear in the comparisons to NOAA-19 SBUV/2 ozone profiles for "chasing" orbits. Adjustments/ corrections are expected for all three by mid-2014.

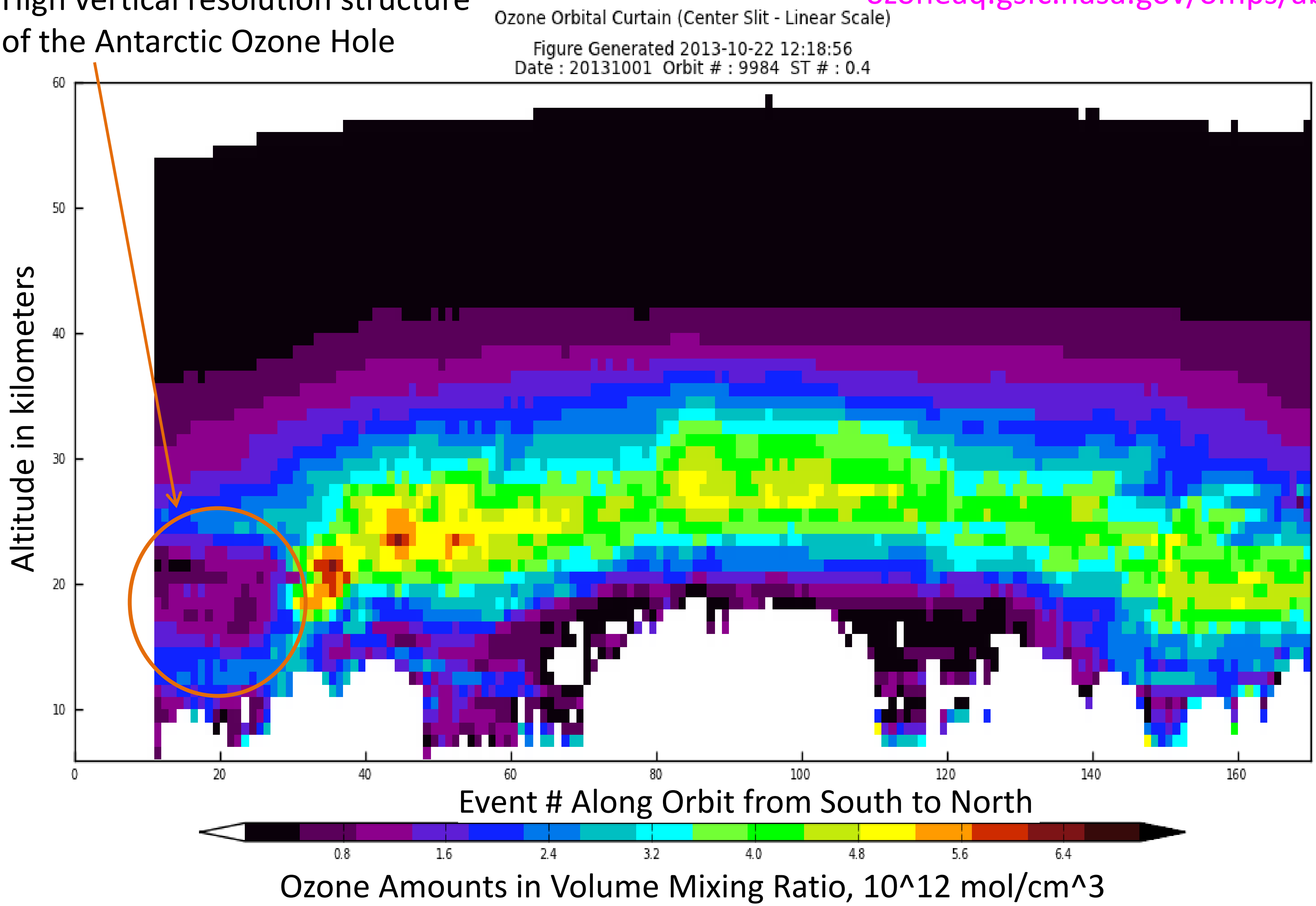
Chasing orbit comparisons of SBUV/2 and OMPS-NP Version 6 Ozone Profiles for July 10, 2013. Figures (a)-(l) show the 12 Umkehr layer amounts versus latitude for the two products. The layer boundaries are given in hPa within the figures. The two orbits are within 50 km and 15 minutes of each other at the Equator.

http://www.star.nesdis.noaa.gov/icvs/prodDemos/proOMPSbeta.O3PRO_IMOPO.php

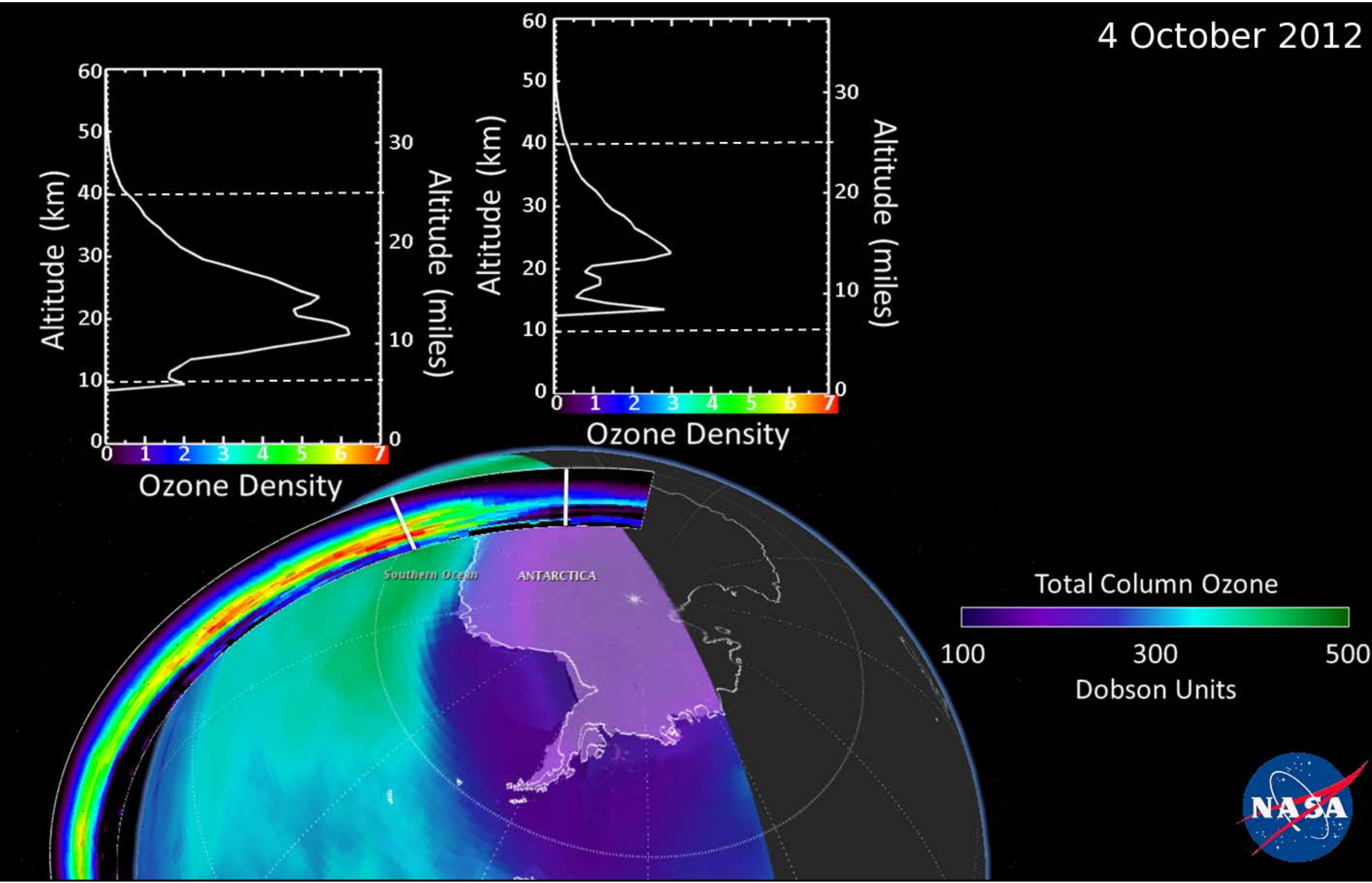
Center Slit, OMPS Limb Ozone Profile Retrievals for one Orbit on October 22, 2013

ozoneaq.gsfc.nasa.gov/omps/about/

High vertical resolution structure of the Antarctic Ozone Hole

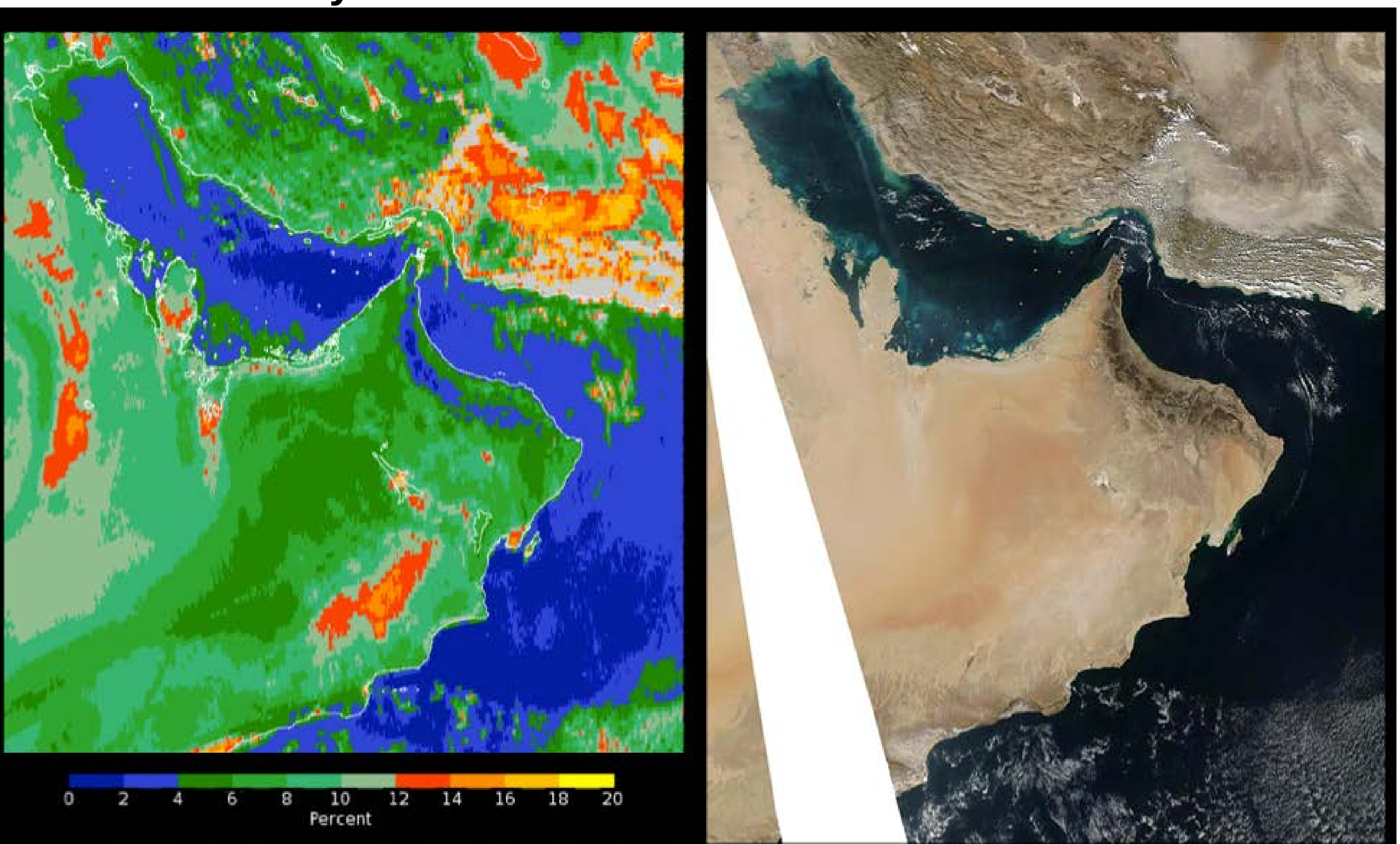


Limb Profiles outside and inside the Antarctic Ozone Hole



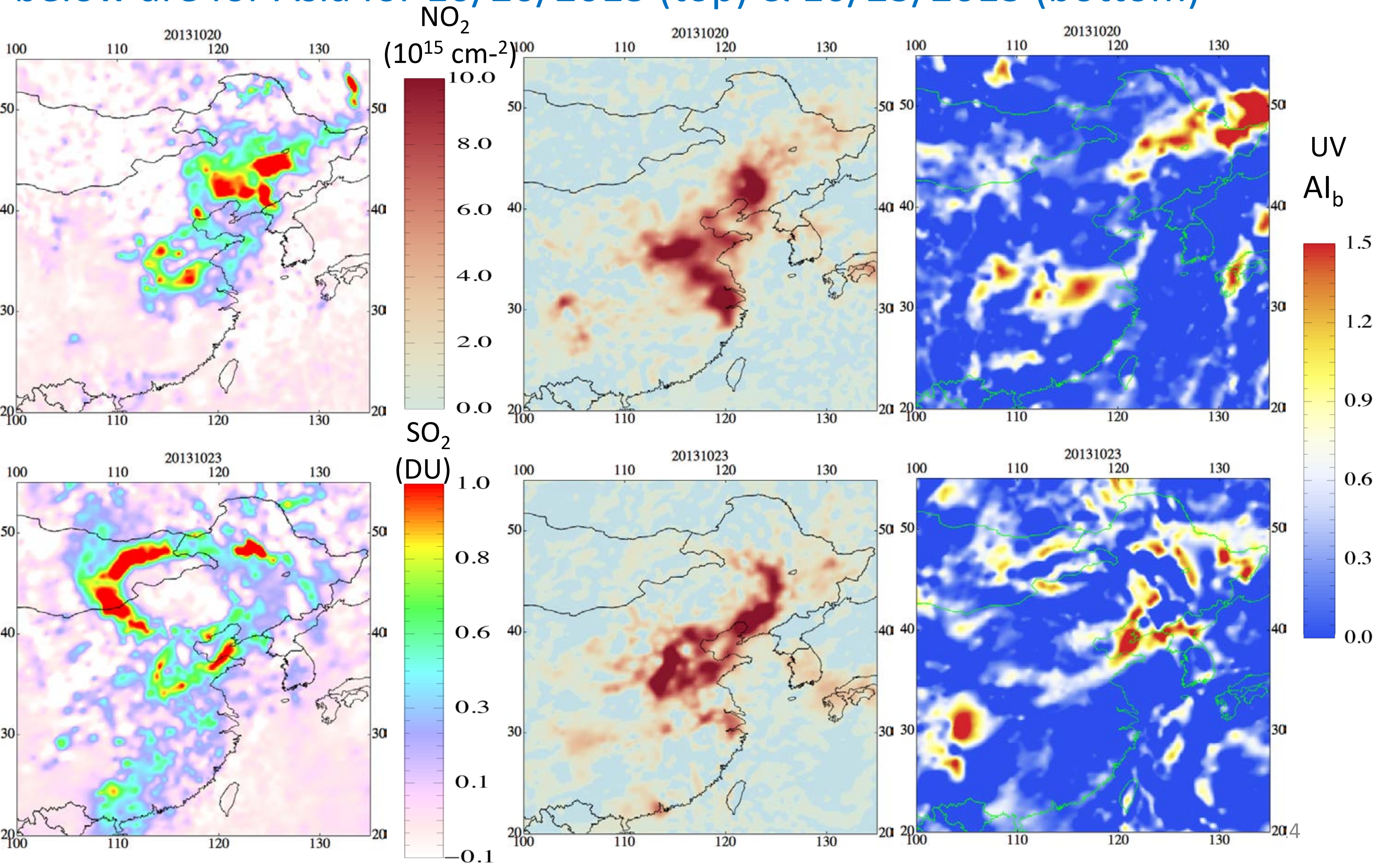
High-Spatial-Resolution Capabilities

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 km² 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.

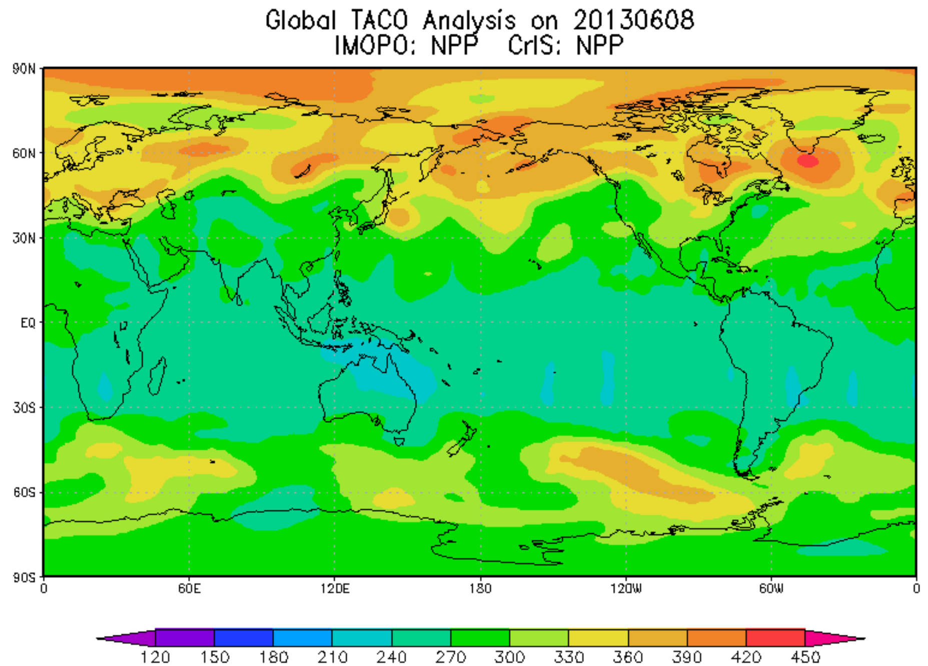


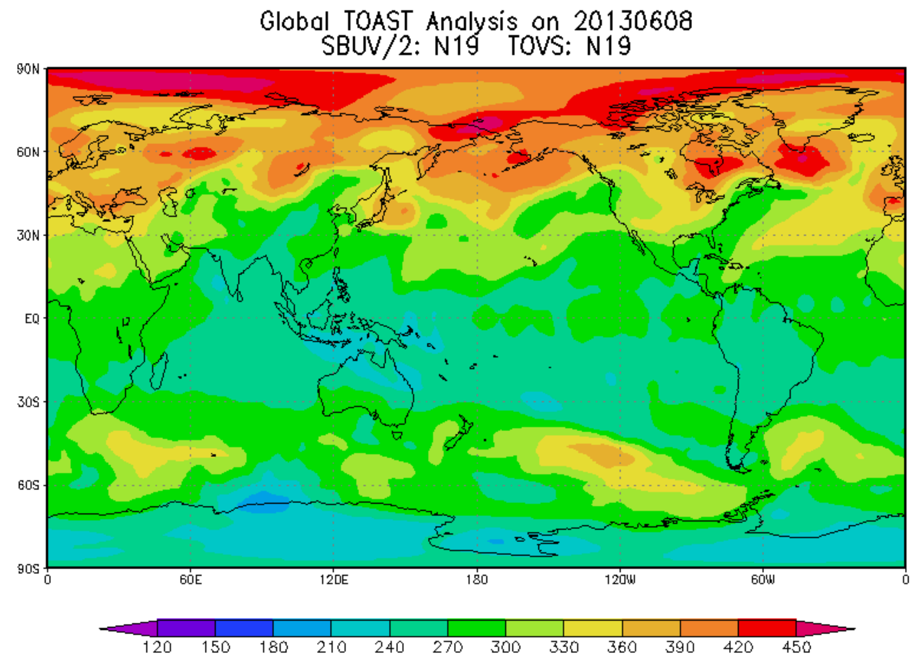
The OMPS Nadir Mapper instrument is very stable, extremely flexible, and has excellent SNRs.

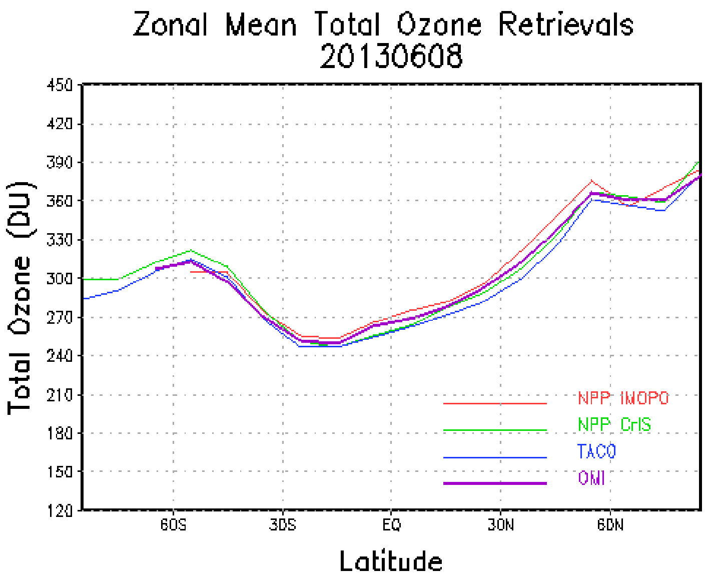
OMPS NM measurements can be used to make state-of-the-art SO_2, NO_2 and Aerosol retrievals for air quality and hazard applications. Examples below are for Asia for 10/20/2013 (top) & 10/23/2013 (bottom)



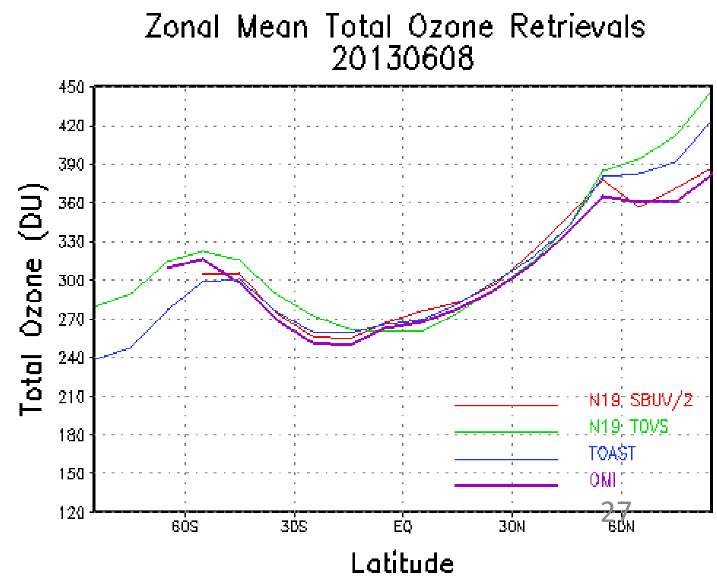
Comparison of TACO (OMPS and CrIS) with TOAST (SBUV/2 and TOVS/HIRS)







Combined products use UV retrievals for the stratosphere and IR retrievals for the Troposphere



Product Summary

- The OMPS instruments are performing well and can deliver ozone products to continue the over 30-years of satellite monitoring.
- Validated nadir total column ozone and ozone profiles will be available operationally by Fall 2014.
- The limb ozone profiles provide global coverage of the ozone layer with high vertical resolution.
- The OMPS measurements can be used to provide other atmospheric chemistry and composition products at good horizontal resolution.

Algorithm Evaluations

NOAA-endorsed algorithm are recommended for use because of legacy, synergy, blended products, performance, maintenance, and other considerations.

Why V8TOz instead of MTTOz?

Provides a set of products consistent with the TOz CDR from the TOMS/SBUV(/2)/OMI record. This also means it can serve as the first step in the CDR cycle of evaluation and reprocessing.

Versions of the algorithm are currently used in OSDPD to make the NOAA GOME-2 NRT TOz products and SBUV/2 TOz products. It is planned for use in making OMPS V8Pro TOz products.

The fundamental ozone estimates are from a single pair of channels simplifying validation studies, calibration adjustments, and anomaly resolution. The MTTOz requires soft calibration of 22 channels.

The V8TOz uses the 313 nm residual to adjust for profile shape variations. The MTTOz was going to use the Limb Profile to do this adjustment.

The V8TOz is synergistic with the Linear Fit SO2 Retrieval algorithm.

Why "I could have had a V8Pro"?

The V8Pro algorithm is in use for the operational and climate data records for the SBUV(/2). It improves on the Version 6 SBUV(/2) algorithm described in Bhartia et al. (1996) as follows:

The V8Pro has a new set of a priori profiles varying by month and latitude, leading to better estimates in the troposphere (where SBUV/2 lacks retrieval information) and allowing simplified comparisons of SBUV/2 results to other measurement systems (in particular, to Umkehr ground-based ozone profile retrievals which use the same a priori data set).

The V8Pro has a true separation of the a priori and first guess. This simplifies averaging kernel analysis. Examples and further information are provided at http://www.star.nesdis.noaa.gov/smcd/spb/ozone/Version8AlgorithmDesc.php

The V8Pro has improved multiple scattering and cloud and reflectivity modeling. These corrections are updated as the algorithm iterates toward a solution.

Some errors present in the V6Pro are reduced. These include the elimination of errors on the order of 0.5% by improved fidelity in the bandpass modeling.

The V8Pro incorporates several ad hoc Version 6 algorithm improvements directly. These include better modeling of the effects of the gravity gradient, better representation of atmospheric temperature influences on ozone absorption, and better corrections for wavelength scale errors.

The algorithm uses improved terrain height information and gives profiles relative to a climatological or forecast surface pressure.

The V8Pro is also designed to allow the use of more accurate external and climatological data and allow simpler adjustments for changes in wavelength selection.

Finally, the V8Pro is designed for expansion to perform retrievals for hyperspectral instruments, such as the Ozone Monitoring Instrument (OMI), the Global Ozone Monitoring Experiment (GOME-2) and the Nadir Profiler in the Ozone Mapping and Profiler Suite (OMPS).

Algorithm Paths Forward

OMPS NP V8Pro (Creates NRT and CDR ozone profiles for SBUV/2)

- A.i. Provide 12 soft calibration adjustments
- A.ii. Change to work with smaller FOVs (just along track)
- A.iii. Put in N-value fitting (Noise reduction, outlier identification and removal, and information concentration)
- A.iv. Add Solar Activity / Scale Factors

OMPS TC V8TOz (Creates NRT and CDR total ozone for GOME-2 and OMI)

- B.i. Provide 12 soft calibration adjustments
- B.ii. Put in Linear-Fit SO2 module. (Eight Granules)
- B.iii. Change to work with smaller FOVs (Interpolate the 35 Cross-track table as needed.)
- B.iv. Put in N-value fitting (Noise reduction, outlier identification and removal, and information concentration)

OMPS LP V2 (Creates high vertical resolution ozone profiles)

- C.i. Continue implementation in NDE
- C.ii. Address aerosol product options

Ozone Products Accomplishments for FY13 to date

- Paper on ozone product performance for Special Issue of JGR
- New DRs:
  - NP/NM FOV Matchup + five distinct scans
  - SZA coverage / orbit start and end of Earth View data
  - Small FOV NM and NP
  - V8TOz
  - SO2 Index and Product
- New CCRs/PCRs:
  - Mixing Fraction limits
  - NM/NP Glueware Correction
- New or Corrected PRO Code provided for IDPS use
  - Change to limit extrapolation of profile shapes
  - Version 8 Profile Retrieval Algorithm \
- Assisting SDR
  - Smear correction
  - measurement-based wavelength scale
  - NM OOB Straylight and NP Straylight corrections
  - new NM and NP SDR wavelength scales and Day 1 solar spectra

Validation and Applications

- Ground-based resources are provided rapidly for match up comparisons.
- Well-characterized satellite measurements are available for additional comparisons via zonal means, chasing orbits, and no local time differences analysis.
- Monitoring results including internal consistency and measurements residual tests are available at www.star.nesdis.noaa.gov/icvs/prodDemos/index.php
- Soft calibration adjustments have been developed and tested for the Version 8 algorithms.
- Users have begun testing provisional products in applications and comparing them to existing products.

(See talks and posters in other sessions.)

Ozone Team Challenges

- Soft Calibration
  Determination and implementation of soft calibration is a moving target as SDR improvements move into the system
- Validation
  Product validation analyses has to be repeated or adjusted as improvements and corrections enter the system.
- Performance versus Schedule issues
  - V8TOz implementation schedule is in competition with V8TOz improvements – SO_2 Linear Fit Algorithm module, small FOVs, Efficiency Factors, Outlier Detection / Information Concentration
  - V8Pro implementation schedule is in competition with V8Pro improvements – Small FOVs, Solar Activity, Outlier Detection / Information Concentration

Background Slides

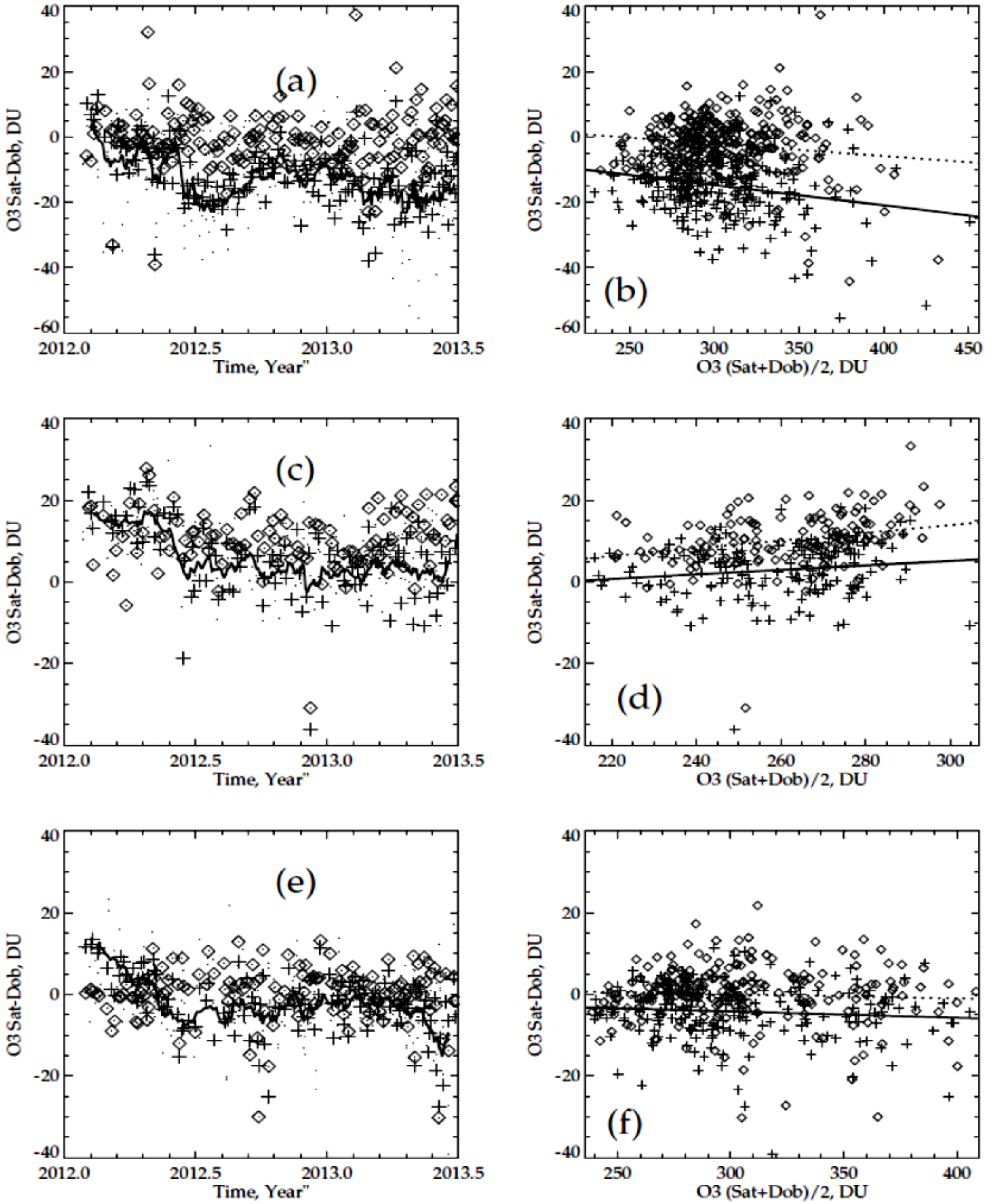


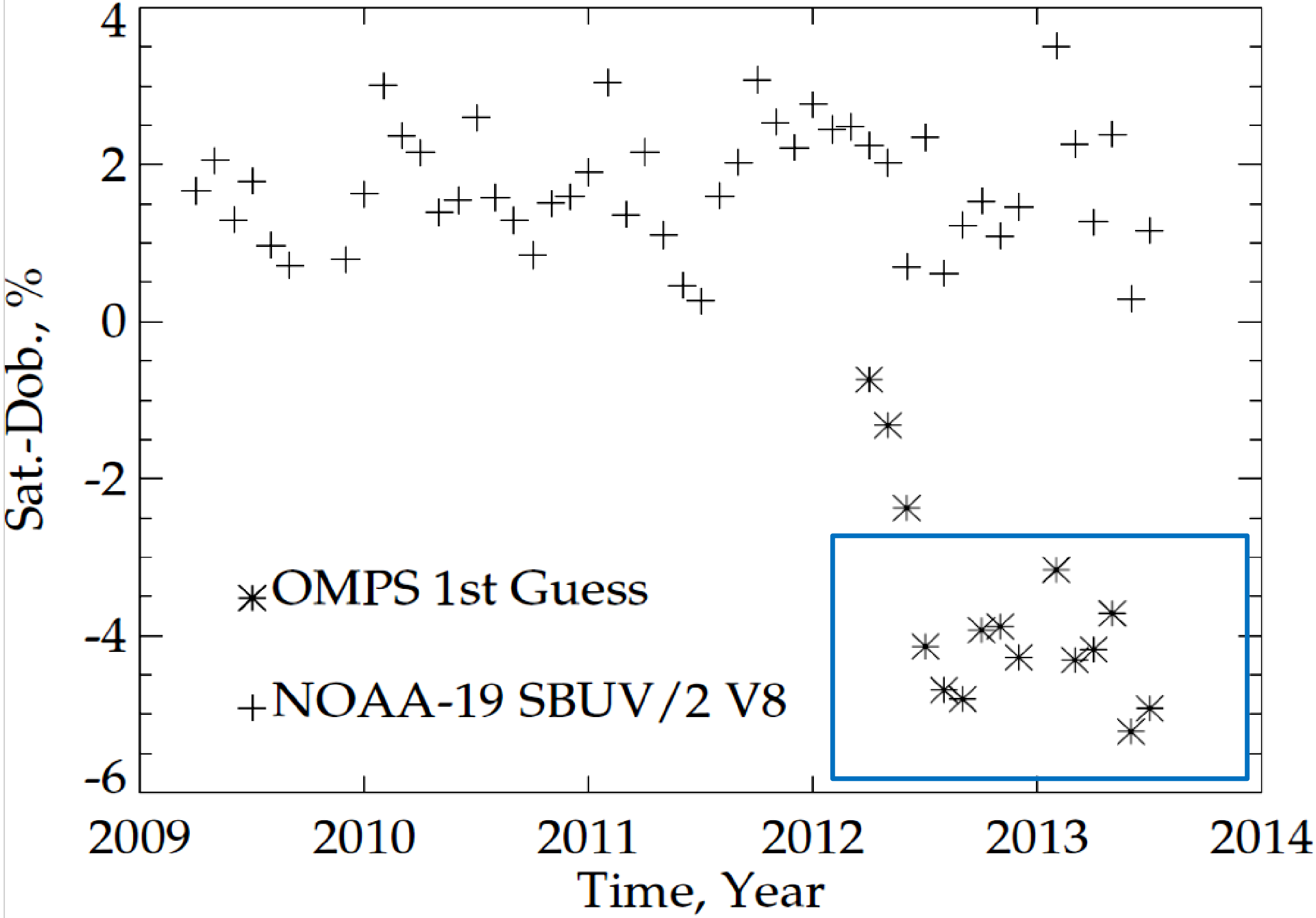
Figure 6. Comparison of OMPS and OMI total column ozone with Dobson estimates for Boulder CO, Manua Loa HI, and Lauder NZ. The figures on the left show the time series of differences for satellite overpass data minus the ground-based Dobson. The diamonds are for OMI and the plus signs are for OMPS. The solid line is the nine-point moving average for the OMPS data. The figures on the right are the satellite minus Dobson differences versus their averages. The solid lines are the linear regression fits for OMPS and the dotted lines are the fits for OMI both with equal noise assumptions. Figure pairs (a) and (b), (c) and (d), and (e) and (f) are for Boulder, Mauna Loa and Lauder, respectively.

Table 1. Statistics for Dobson Match-Up Data Sets In Figure 6.

Site # Days	Sat. Name	**Avg_G** DU	**Avg_S** DU	**m_G**	**m_S**	**m_E**	**σ**	**δ** DU	**ε** DU	**ρ**	**Min_E** DU	**Max_E** DU
BOU	OMPS	308.7	293.9	0.90	0.98	0.94	0.02	6.7	6.3	0.97	-10.6	-24.1
N=335	OMI	308.7	306.3	0.93	1.00	0.96	0.02	6.4	6.1	0.97	0.3	-8.1
MLO	OMPS	256.6[c]	259.4	0.99	1.13	1.06	0.03	4.7	4.9	0.93	0.4[c]	5.9[c]
N=217	OMI	256.6[c]	266.9	1.03	1.17	1.10	0.03	4.4	4.8	0.94	6.0[c]	15.6[c]
LAU	OMPS	304.5	300.2	0.97	1.00	0.99	0.02	4.8	4.7	0.99	-3.3	-5.8
N=270	OMI	304.5	304.4	0.97	1.01	0.99	0.02	5.3	5.2	0.98	0.6	-1.1

[c]The Dobson station is near the top of Mauna Loa. Satellite FOVs include ocean scenes. Adjustments from 6 to 12 DU have been used to account for these scene differences based on Hilo HI ozonesondes and standard ozone profiles.

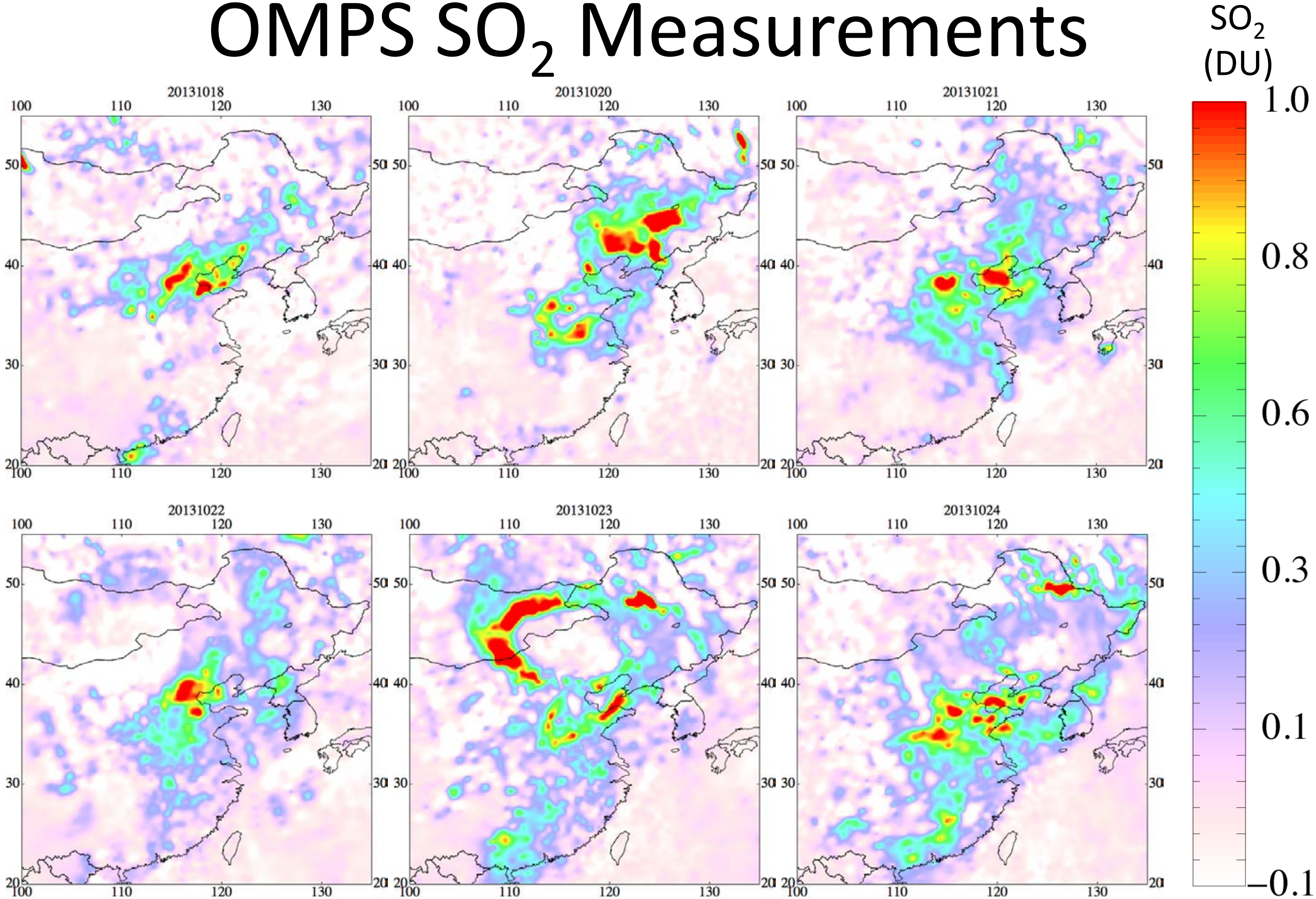
The OMPS Bias estimates at the maximum and minimum data values for each station show negative biases.



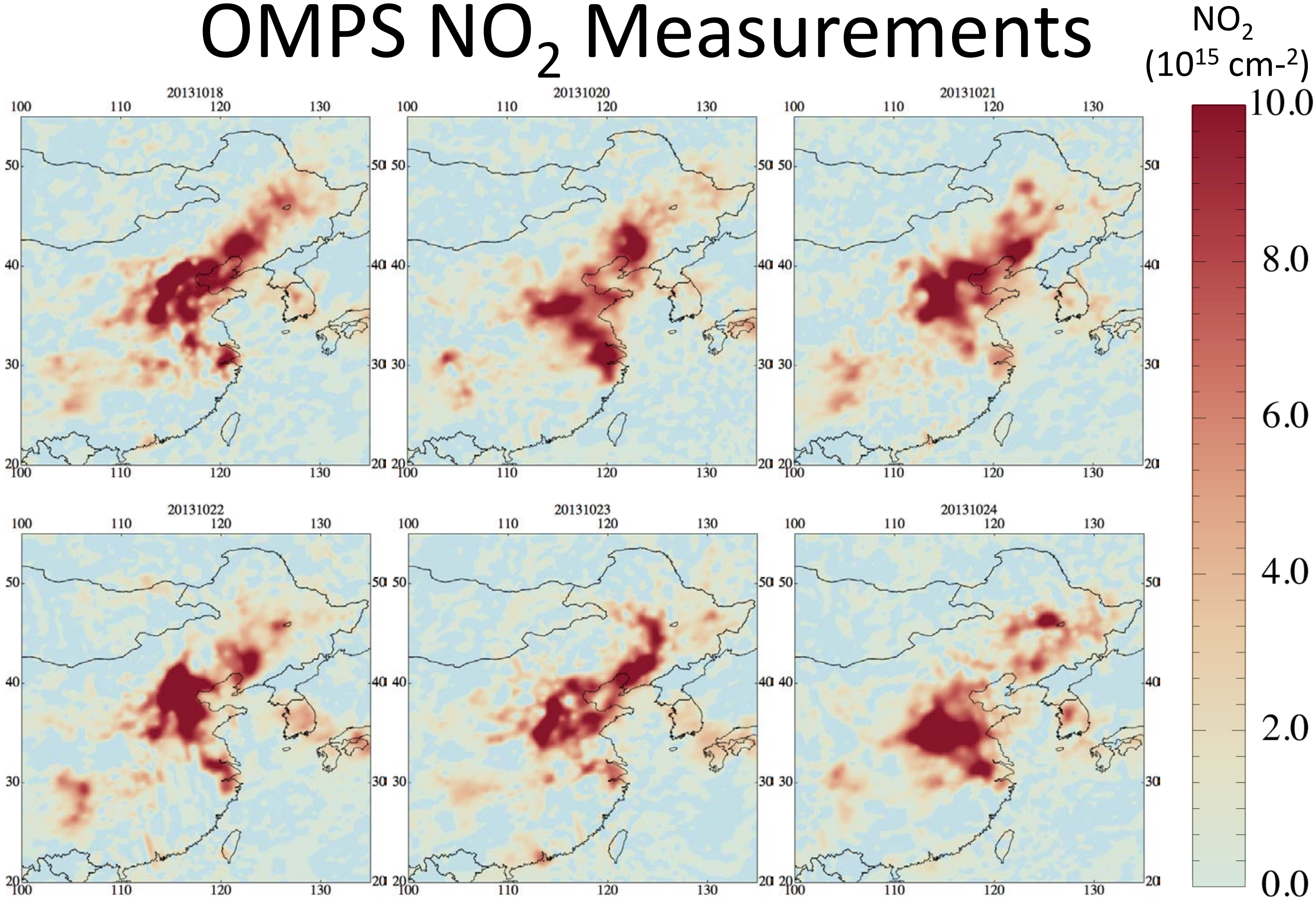
Another view of the negative overall bias in the OMPS TOZ relative to ground-based Dobson Station estimates.

Figure 7. Monthly differences between matchup NOAA-19 SBUV/2 Version 8 total column ozone and OMPS 1st Guess total column ozone with a collection of Dobson observations from 22 stations from the World Ozone Data Center. For OMPS, the data are distance-weighted averages for estimates within 0.5º Latitude and SEC(Latitude)º Longitude of each station's location. For SBUV/2, the data are distance-weighted averages for estimates within 2.0º Latitude and 20º Longitude of each station's location. Each data point is a monthly average difference for the satellite instrument versus the Dobson ones. At least six matchup values are required for a station to be used in the monthly average. As few as five stations may have reported enough data for the later values.

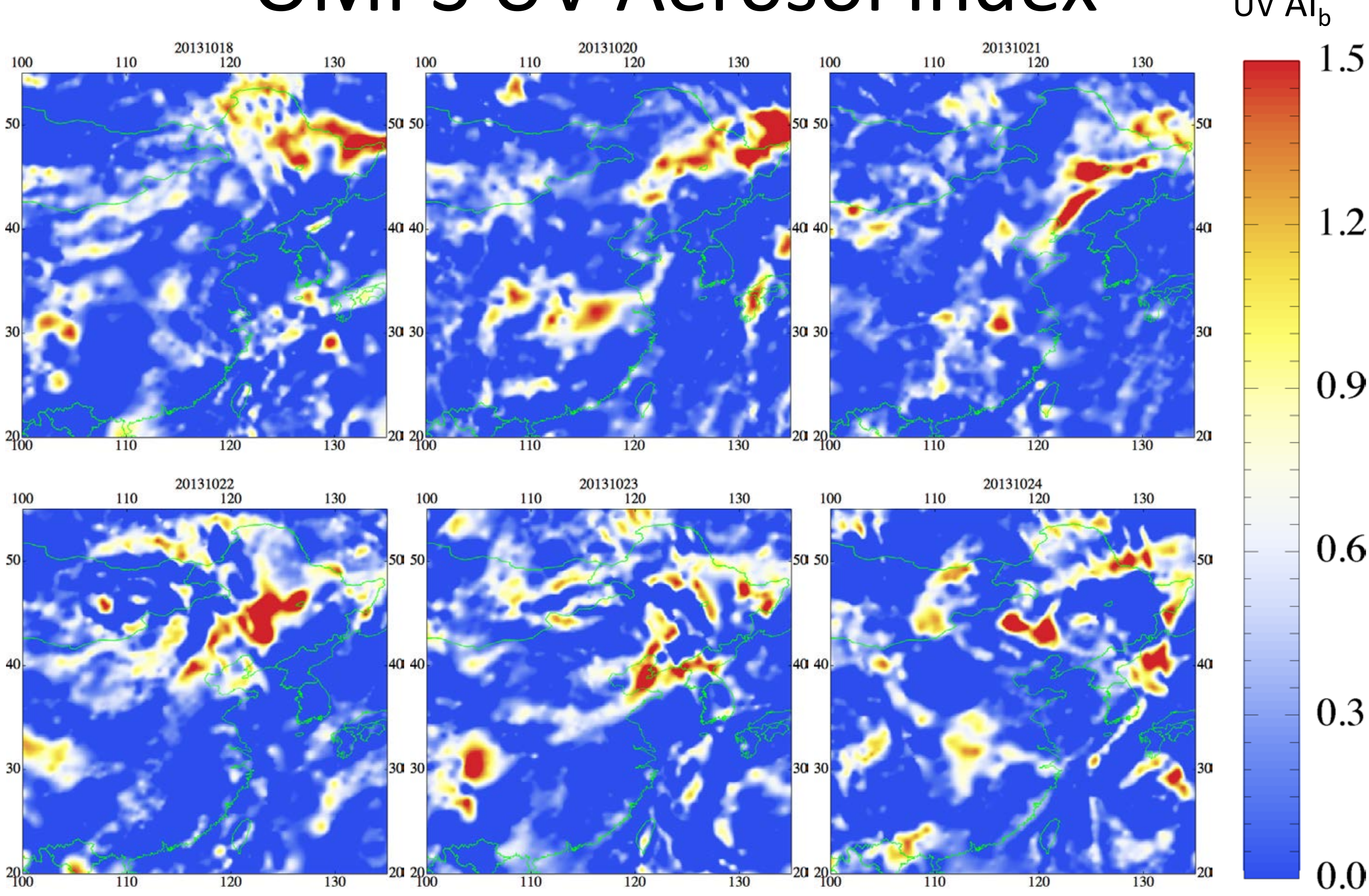
OMPS SO_2 Measurements



OMPS NO_2 Measurements



OMPS UV Aerosol Index



Nadir Mapper / Total Ozone Key Points

- The OMPS NM SDR needs calibration adjustments (consistent with the intra-orbit wavelength scale adjustments) to reduce offsets with other products and to remove cross-track biases.
- A new day 1 solar with a wavelength scale in the middle of the Earth-view range would give better results.
- A better Out-of-Range Stray Light correction could help to resolve the Nadir Profiler SDR characterization between 300 nm & 310 nm.
- The OMPS NM SDR can be used to provide a range of atmospheric composition product at high resolution.

Ozone Profile Product, **IMOPO**

The spectral measurements from the OMPS Nadir Profiler and Nadir Mapper of the radiances scattered by the Earth's atmosphere are used to generate estimates of the ozone vertical profile along the orbital track (**IMOPO**). The algorithm uses ratios of Earth radiance to Solar irradiance at a set of 12 wavelengths (at approximately 252, 273, 283, 288, 292, 298, 302, 306, 313, 318, 331 and 340 nm) with eight from the Nadir Profiler and four from the Nadir Mapper to obtain estimates of the total column ozone, effective reflectivity, and the ozone vertical profile in 12 Umkehr Layers. The radiances for the four longer wavelength are obtained from the 25 Nadir Mapper FOVs co-located with a single Nadir Profiler FOV. The longer channel radiance/irradiance ratios are used to generate estimates of the total column ozone and scene effective reflectivity. The total column ozone is used to generate a first guess ozone profile that becomes the A Priori for a maximum likelihood ozone profile retrieval using the ratios for the seven shortest wavelengths (omitting the 253 nm channel and including 313 nm at high SZA). Additional information is in the OMPS Nadir Profile Algorithm Theoretical Basis and Operational Algorithm Description Documents, and a volume of the Common Data Format Control Book at:
http://npp.gsfc.nasa.gov/documents.html

OMPS NP ATBD 474-00026_Rev-Baseline.pdf

OMPS NP OAD 474-00067_OAD-OMPS-NP-IP-SW_RevA_201

Intermediate Product CDFCB

474-00001-04-01_CDFCB-Vol4-Part1_Rev-_Block-1-1_31Mar2011.pdf20127.pdf

Instrument Performance – NP

Requirement	Specification/Prediction Value	On-Orbit Performance
Non-linearity	< 2% full well	< 0.46%
Non-linearity Knowledge	< 0.5%	~0.1%
On-orbit Wavelength Calibration	< 0.01 nm	
Stray Light NM Out-of-Band + Out-of-Field Response	≤ 2	average ~± 2%*
Intra-Orbit Wavelength Stability	<0.02 nm	< 0.013 nm
SNR	Channel Dependent	Similar to SBUV/2 at corresponding channels^
Inter-Orbital Thermal Wavelength Shift	<0.02 nm	0.03 nm annual cycle#
^CCD Read Noise	<60 –e RMS	< 25 –e RMS
Detector Gain	>43	~45
Absolute Irradiance Calibration Accuracy	< 7%	1~10% , average: ~7%
Absolute Radiance Calibration Accuracy	< 8%	< 5%

* A measurement-based correction using prelaunch characterization will improve accuracy and precision

Regular annual cycle affects accuracy and stability

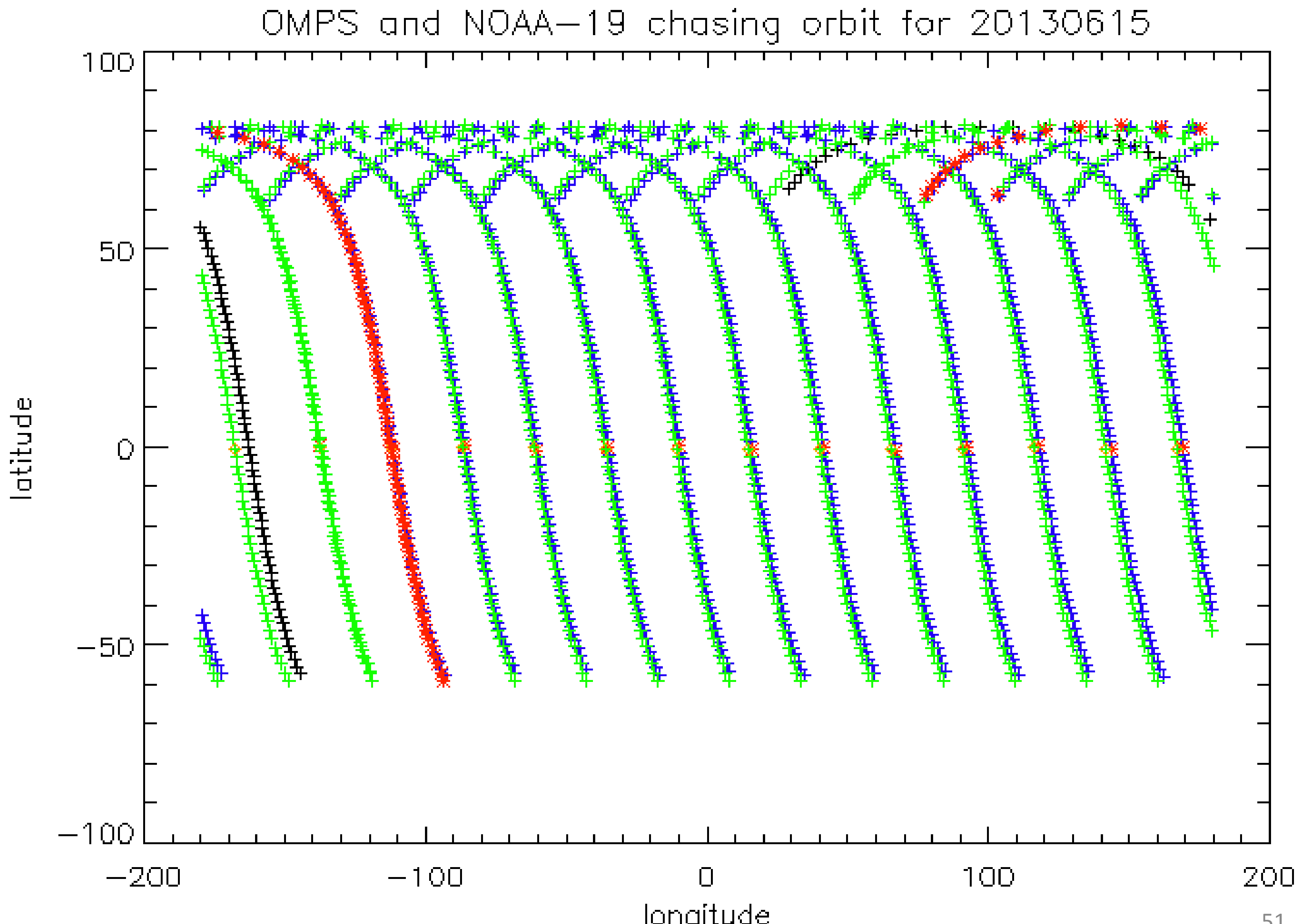
^ Information concentration possible by using near-by channels.

C. Pan

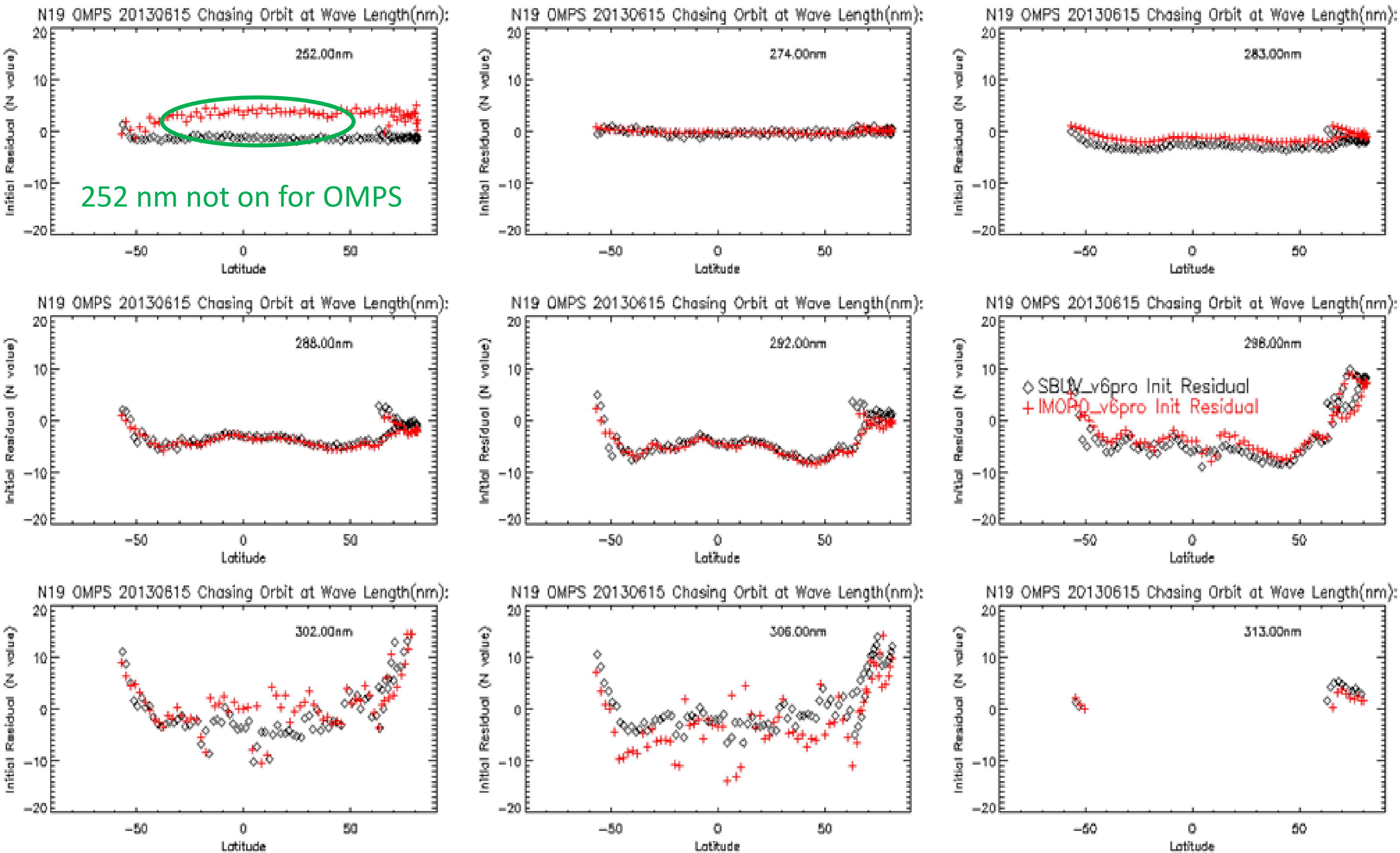
Profile comparisons between OMPS & SBUV/2 V6Pro

The figures on the next four slides show comparisons of the ozone profile retrievals estimates between IMOPO and the NOAA-19 SBUV/2 processed with the Version 6 ozone profile retrieval algorithm. The data are from another single pair of orbits on June 15, 2013 where the two satellites are flying in formation (orbital tracks within 50 KM and sensing times with 10 minutes). The first of the four slides shows the orbital tracks. The second compares the initial measurement residuals at the nine profiling wavelengths.
The third compares the ozone profile retrievals in 12 pressure layers in Dobson Units versus Latitude. The 12 layers are defined by the following 13 layer boundaries: [0.0,0.247,0.495,0.99,1.98,3.96,7.92,15.8,31.7,63.3,127.0,253.0,1013] hPa.
The top three layers' results are in the top row with the topmost layer on the upper left. The lowest layer's results are in the figure on the bottom right. The OMPS Nadir Profiler values are in Red and the **SBUV/2 are shown in Black**. A significant number of the OMPS Nadir Profilers contain fill values because of Error Codes incorrectly set to 20.
The fourth shows the results of comparison for the ozone mixing ratios at 19 pressure levels: [0.3,0.4,0.5,0.7,1.0,1.5,2.0,3.0,4.0,5.0,7.0,10.,15.,20.,30.,40.,50.,70.,100.] hPa. The arrangement from top to bottom follows the same convention as for the layers.
The two last sets of figures show similar results with general agreement between the retrievals for the two instruments but with the OMPS NP retrieving much smaller values at the top of the profiles. This is due to the inaccuracies in the initial calibration of the shorter wavelength channels and out-of-band of stray light in the shorter wavelength channels providing information at those levels.

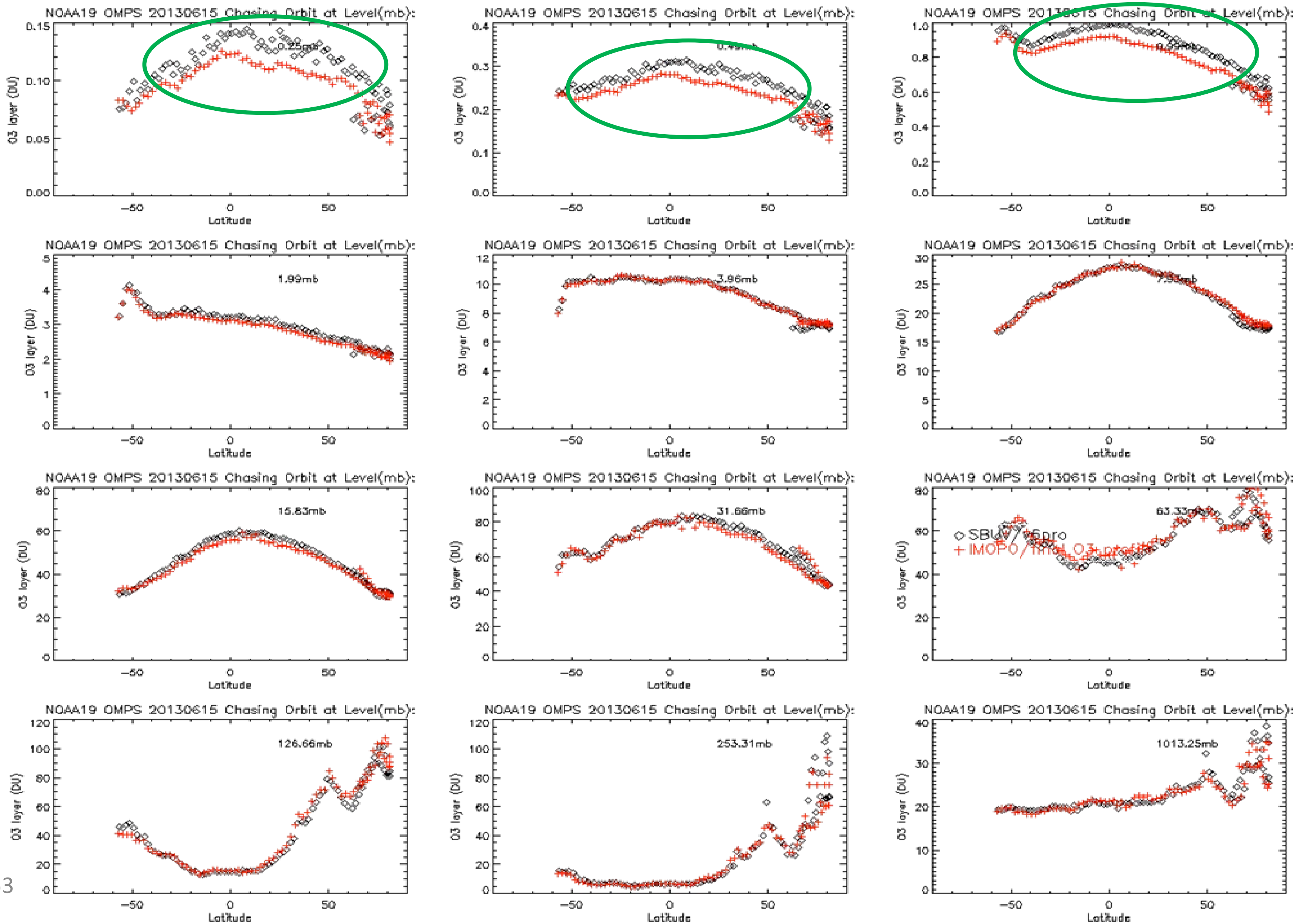
Well-matched Orbits for June 15, 2013

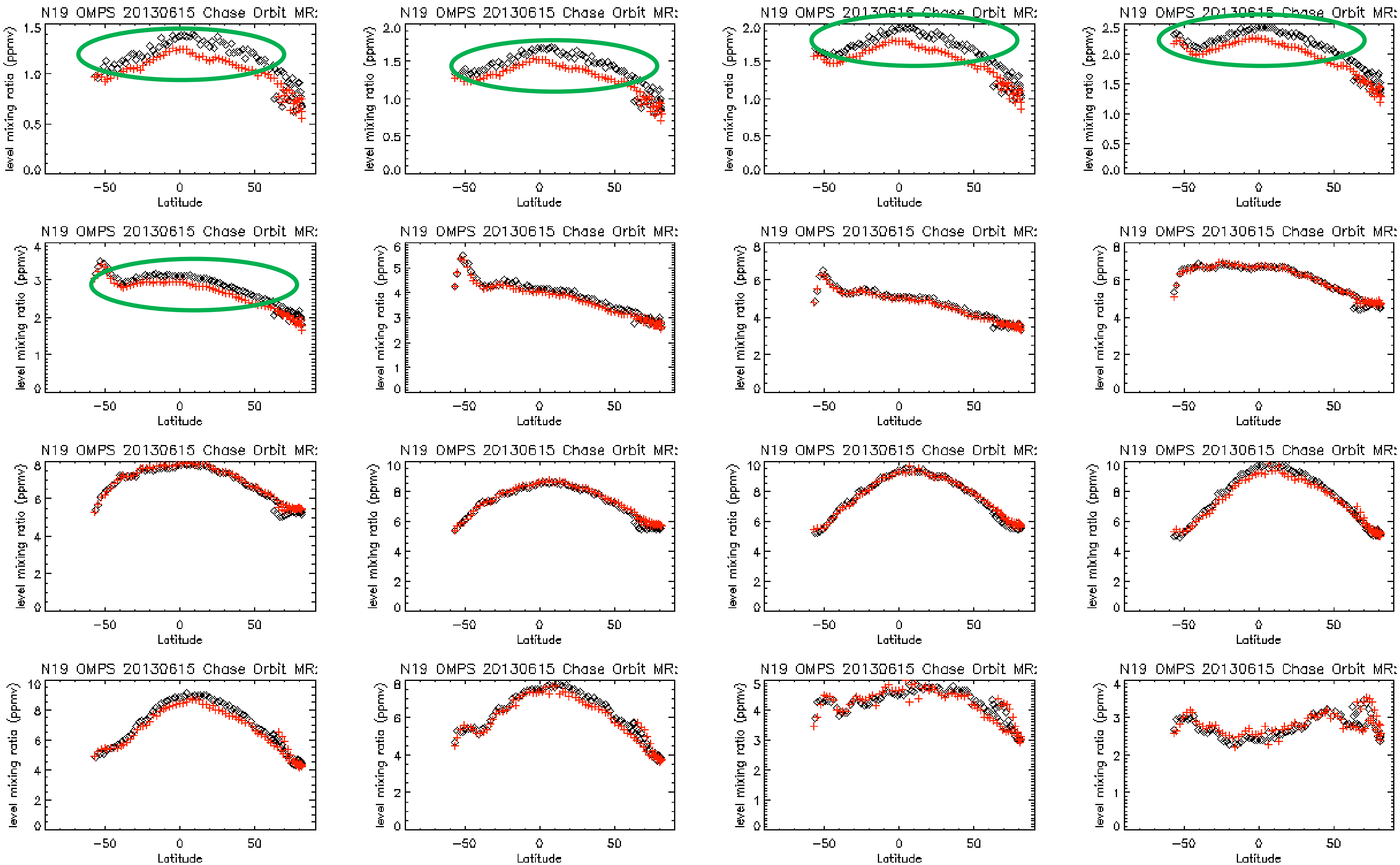


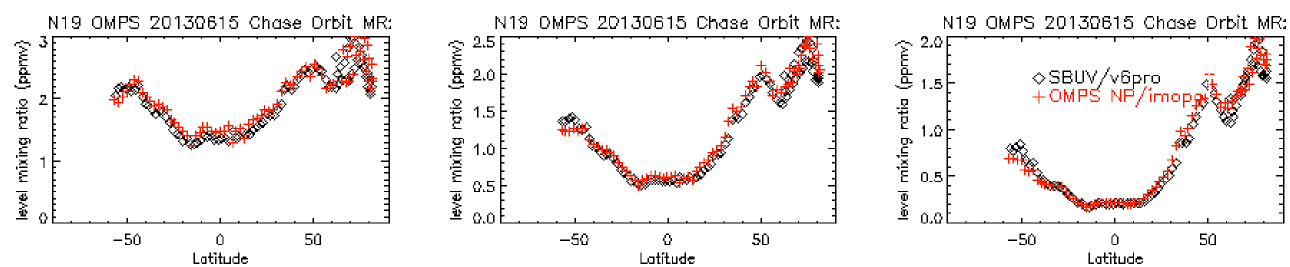
Comparison of Initial V6 Measurement Residuals for S-NPP OMPS NP and NOAA-19 SBUV/2



Chasing orbit comparisons of SBUV/2 & OMPS-NP Version 6 Ozone Profiles







Upper layers are most affected by stray light and 252 nm channel use.

[0.3,0.4,0.5,0.7,1.0,1.5,2.0,3.0,4.0,5.0,7.0,10.,15.,20.,30.,40.,50.,70.,100.] hPa.

Total Column Ozone* Products

The spectral measurements from the OMPS Nadir Mapper* of the radiances scattered by the Earth's atmosphere are used to generate estimates of the total column ozone. The algorithm uses ratios of Earth radiance to Solar irradiance at triplets of wavelengths to obtain estimates of the total column ozone, effective reflectivity, and the wavelength dependence of the reflectivity. Table values computed for a set of standard profiles, cloud heights, latitudes and solar zenith angles are interpolated and compared to the measured top-of-atmosphere albedos. The triplets combine an ozone insensitive wavelength channel (at 364, 367, 372 or 377 nm) to obtain cloud fraction and reflectivity information, with a pair of measurements at shorter wavelengths. The pairs are selected to have one "weak" and one "strong" ozone absorption channel. The hyperspectral capabilities of the sensor are used to select multiple sets of triplets to balance ozone sensitivity across the range of expected ozone column amounts and solar zenith angles. The "strong" ozone channels are placed at 308.5, 310.5, 312.0, 312.5, 314.0, 315.0, 316.0, 317.0, 318.0, 320.0, 322.5, 325.0, 328.0, or 331.0 nm. They are paired with a longer "weak" channel at 321.0, 329.0, 332.0, or 336.0 nm. The ozone absorption cross-sections decrease from 3.0 $(atm.\ cm)^{-1}$ to 0.3 $(atm.\ cm)^{-1}$ over the range of "strong" wavelengths. Typical ozone columns range from 100 DU or 0.1 atm-cm to 600 DU or 0.6 atm-cm.

*There is sometimes confusion on what to call the OMPS instruments and products. The OMPS Nadir Mapper (NM) makes the principal measurements that are used to create the Total Column Ozone (TC or TOZ) Products.

The 1st Guess Total Ozone Product INCTO

The Multiple Triplet algorithm described in the previous slide is applied twice for each FOV. This was done to resolve the "Who goes first?" problem created by the desires to use information from other sensors in the retrieval algorithms, e.g., OMPS wanted to use the CrIS temperature profile, and CrIS wanted to use the OMPS ozone estimates. The "1st Guess" OMPS products (**INCTO**) use climatological or forecast fields for surface reflectivity and pressure, snow/ice coverage, cloud optical centroid depth, and atmospheric temperature. They use internally calculated estimates of cloud fractions and effective reflectivity from measurements at non-ozone absorbing UV wavelengths. As we will show, this application of the algorithm is performing well. This product is sometimes called the Total Ozone First Guess Intermediate Product (TOZ IP).

REFERENCES – Additional information is in the OMPS Total Column Algorithm Theoretical Basis and Operational Algorithm Description Documents, and a volume of the Common Data Format Control Book:
Available at http://npp.gsfc.nasa.gov/documents.html
OMPS Total Column Ozone ATBD 474-00029_Rev-Baseline.pdf
OMPS Total Column Ozone OAD 474-00066_OAD-OMPS-TC-EDR-SW_RevA_20120127.pdf
Atmospheric EDRs CDFCB 474-0001-04-02_Rev-Baseline.pdf

The 2nd Pass Total Ozone Product, OOTCO

The "2nd Pass or EDR" OMPS products (**OOTCO**) use the same UV cloud top pressures as INCTO but obtain snow/ice coverage from VIIRS near-real-time products and temperature profiles from CrIMSS products. The products use the same logic as INCTO to internally calculated estimates of cloud fractions and effective reflectivity from measurements at non-ozone absorbing UV wavelengths. As we will show, this application of the algorithm is performing well. This product is sometimes called the Total Ozone Environmental Data Record (TOZ EDR). The INCTO and OOTCO products use identical sets of measurements from the OMPS Nadir Mapper. The INCTO final ozone estimate is included as a parameter in the OOTCO output files.

REFERENCES – Additional information for this product is available in the documents listed for INCTO on the previous slide.

Nine Things to Know about the OMPS Total Ozone EDR

- The algorithm uses information at 22 wavelengths obtained from 44 macropixels (20 or more pixels) x 35 cross-track measurements
- Channels are combined three at a time to generate ozone, reflectivity and wavelength dependence of reflectivity (e.g., aerosol effects) estimates
- A single triplet is used to generate the heritage Version 7 ozone estimate
- A single triplet is used to generate the SO2 Index. It shows the effect of inter-channel biases and its use is problematic at high Solar Zenith Angles.
- Internal comparisons monitoring cross-track variations in ozone, reflectivity, aerosol and SO2 Index values provide direct information on inter-channel biases
- Absolute calibration of the reflectivity channels is tested by vicarious methods by using Greenland and Antarctic ice fields, cloud-free equatorial Pacific ocean, and minimum land values.
- Absolute calibration of ozone sensitive channels can be set to agree with the validation "truth" data set of choice.
- The First Guess IP and EDR products have been converging.
  - Partial Cloud calculations are the same except for the use of differing Snow/Ice information
    - Identical logic for cloud fractions and input for cloud top pressures
    - Snow/Ice for NRT VIIRS in EDR is still erroneous – improvements in the pipeline
    - Snow/Ice tilings in 1st Guess are better than climatology; will be daily starting in 2014
  - Temperature data options – Climatology, NCEP, CrIMSS (and correction On/Off)
    - Need to bring forecasts for the stratosphere into IDPS and turn on the correction for the IP.
  - Profile mixing fraction is problematic when it extrapolates (DR7310/CCR)
- The total ozone column products do not currently meet precisions requirements. Wavelength scale knowledge and soft calibration adjustments to remove inter-channel and cross-track calibration errors in the SDR are necessary to achieve the performance.

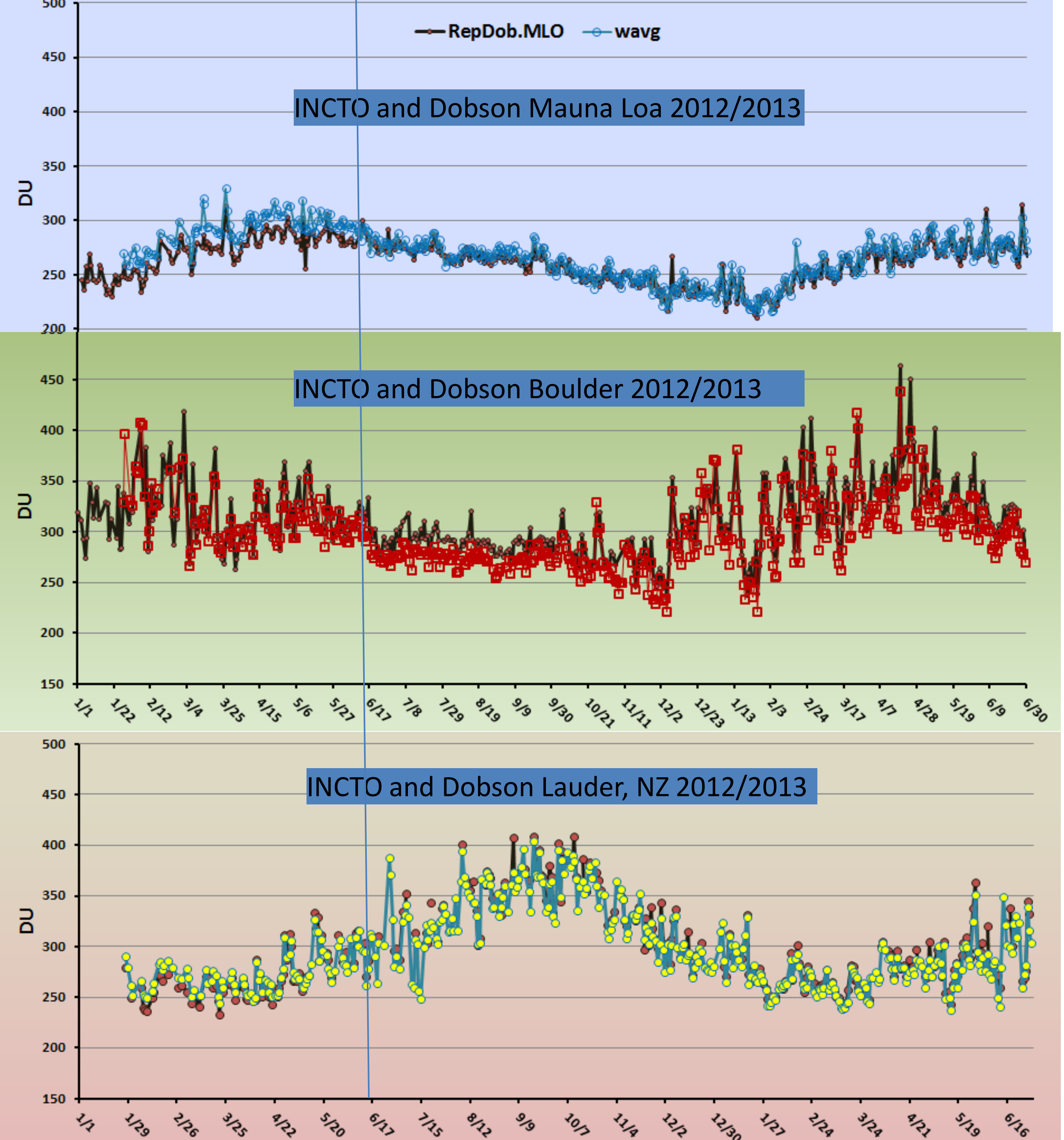
Instrument Performance – OMPS NM at Provisional

Requirement	Specification/Prediction Value	On-Orbit Performance
Non-linearity	< 2% full well	< 0.46%
Non-linearity Knowledge	< 0.5%	~0.1%
On-orbit Wavelength Calibration	< 0.01 nm	average ~0.01 nm RMS
Stray Light NM Out-of-Band + Out-of-Field Response	≤ 2	average ~± 2%^
Intra-Orbit Wavelength Stability	<0.02 nm	< 0.013 nm*
SNR	>1000	> 1000 from SV and EV
Inter-Orbital Thermal Wavelength Shift	<0.02 nm	<0.013 nm
CCD Read Noise	<60 –e RMS	< 25 –e RMS
Detector Gain	>46	~42
Absolute Irradiance Calibration Accuracy	< 7%	5%
Absolute Radiance Calibration Accuracy	< 8%	< 5%

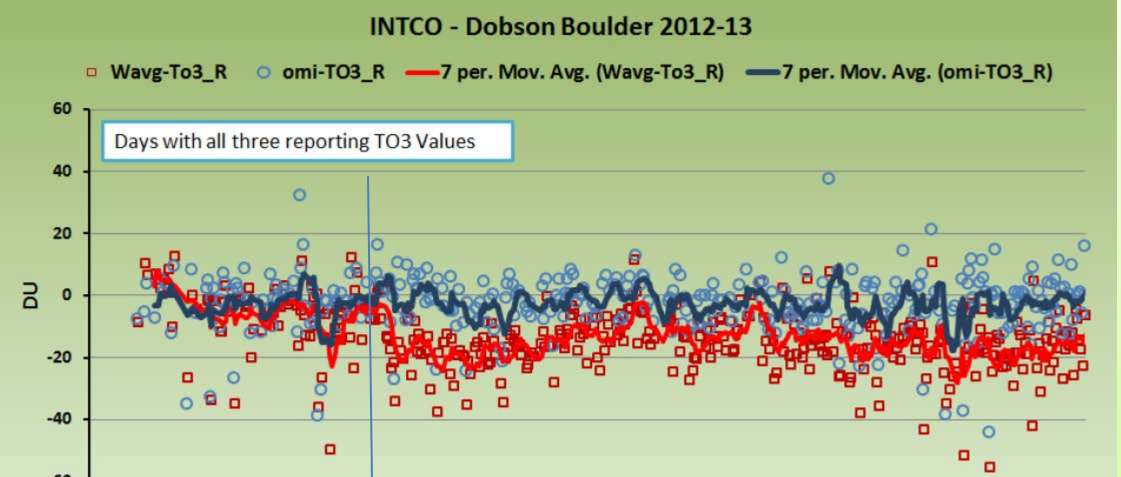
^ Need 0.5% pixel to pixel for triplet wavelengths after measurement-based correction.

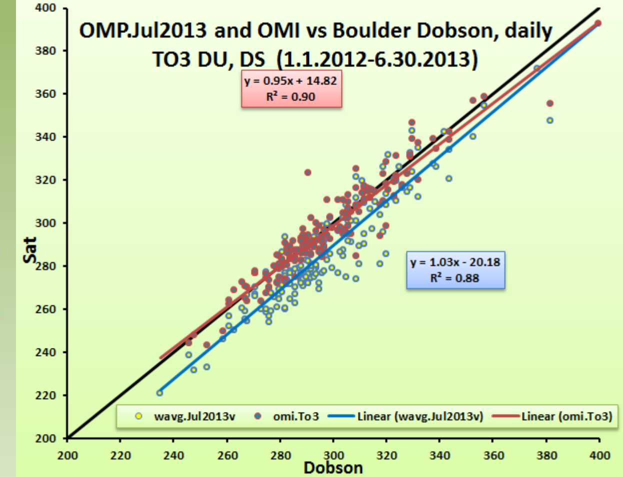
* New results show need for intra-orbit adjustments to reach this perfomance.

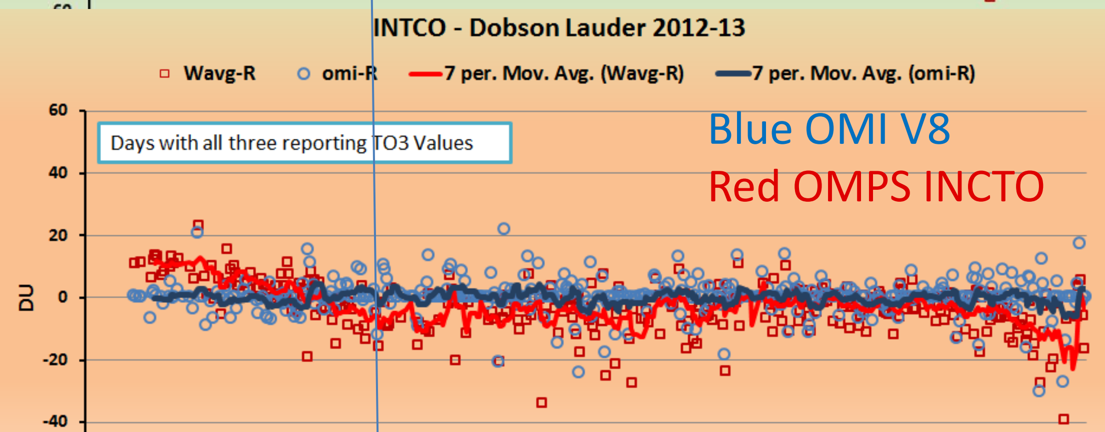
C. Pan



Comparisons of INCTO to three very good Dobson ground stations 1/2012 to 6/2013. Notice the shift in biases in June 2012 with the introduction of new solar flux and wavelength scales.

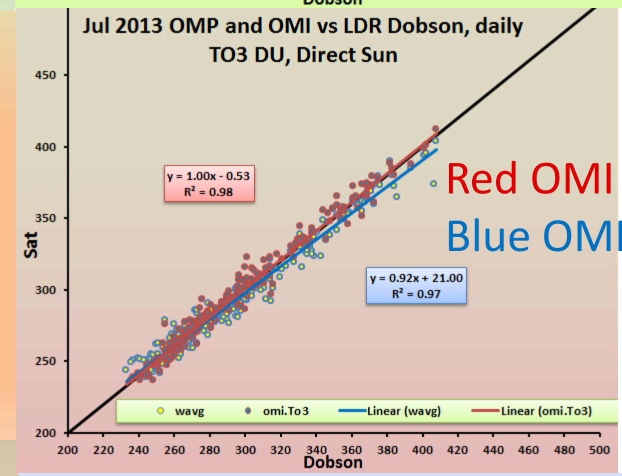






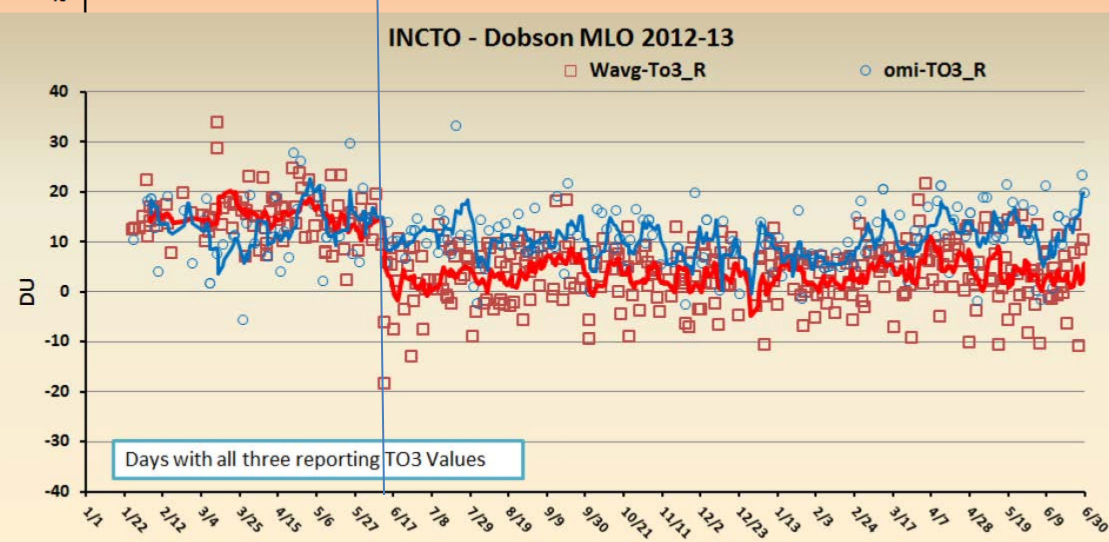
Blue OMI V8

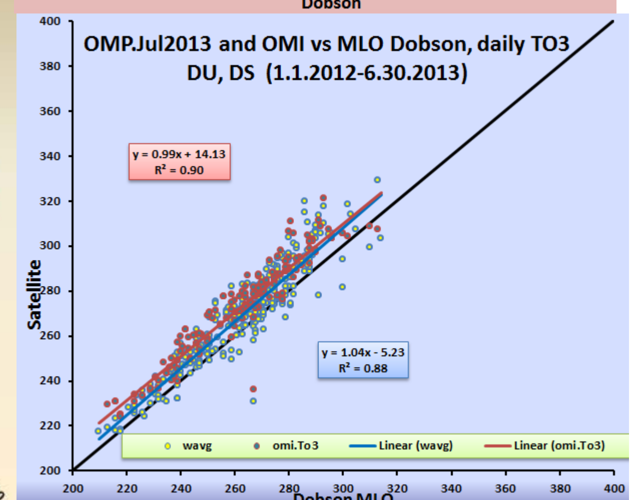
Red OMPS INCTO



Red OMI V8

Blue OMPS INCTO

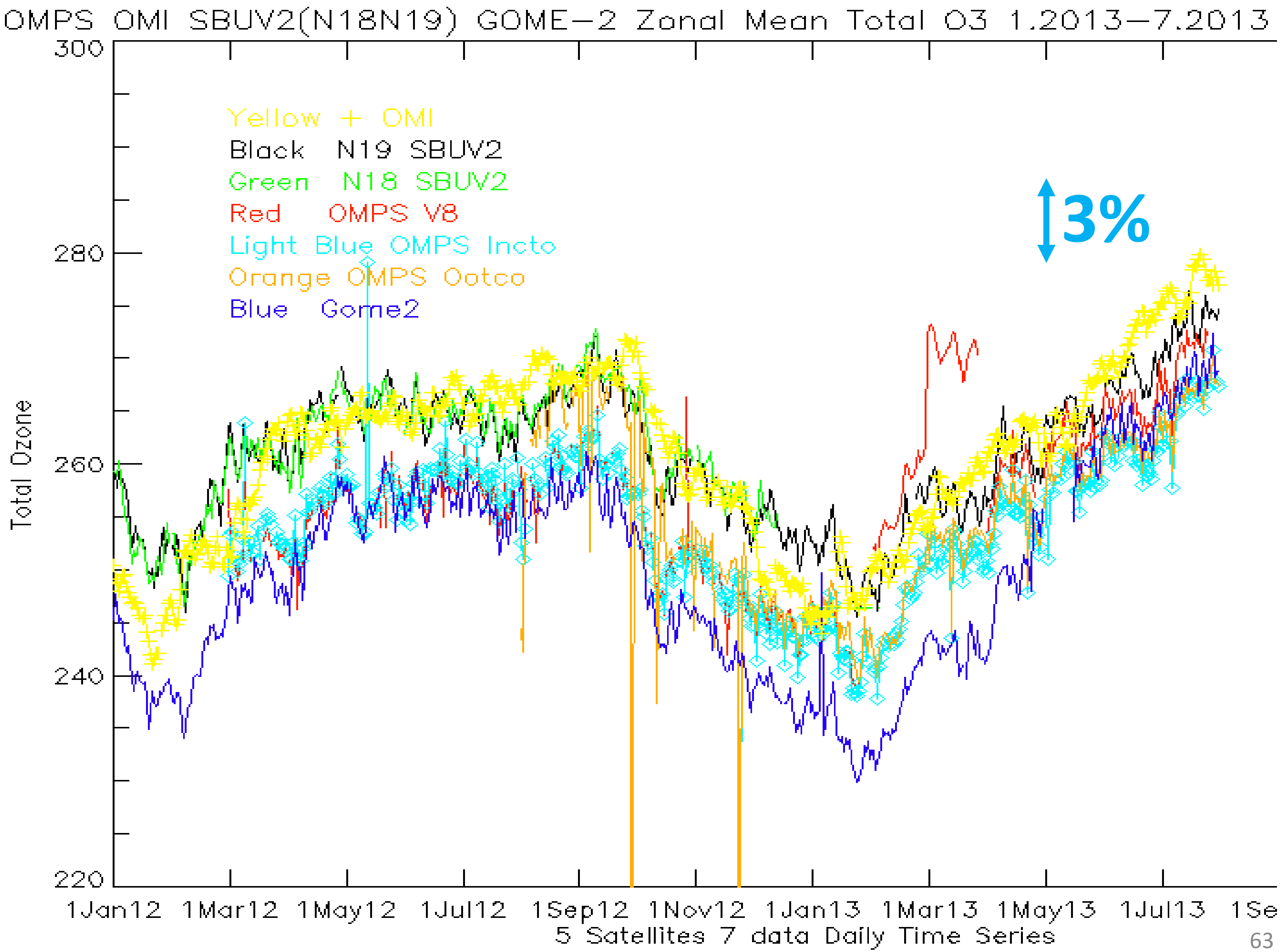




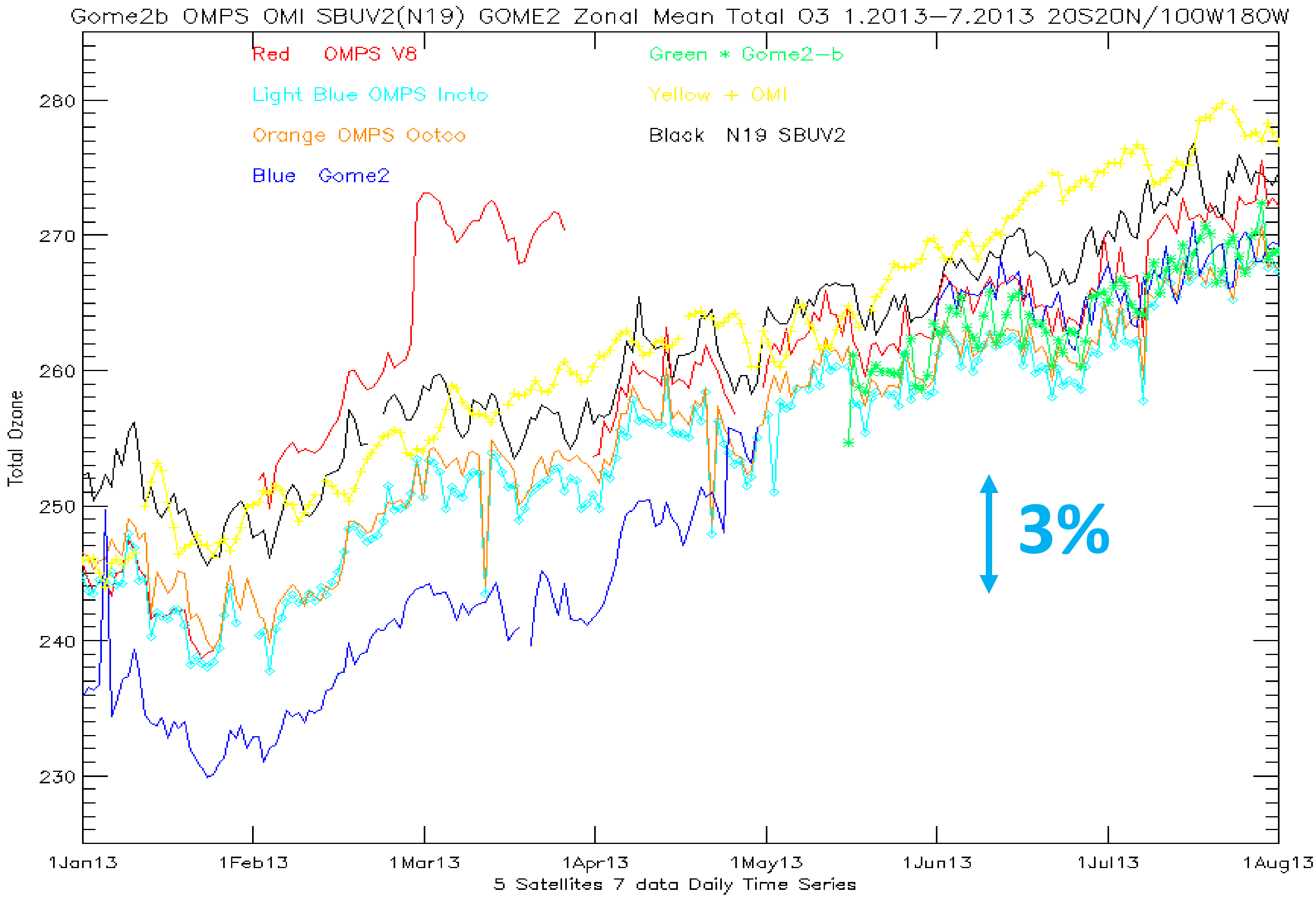
Time Series of Equatorial Pacific zonal means for INCTO and OOTCO versus other satellite measurements

- The next slide shows time series of zonal means for ozone estimates from NOAA-18 and NOAA-19 SBUV/2, MetOp-A GOME-2, NASA EOS Aura OMI and JPSS S-NPP OMPS INCTO, OOTCO and V8. The SBUV/2 and GOME-2 estimates are from Version 8 algorithms. The GOME-2 has not been adjusted for known degradation in the scan mirror until the end of the record.
- The figure on the first slides shows a bias of ~3% between the OMPS and SBUV/2 products. This is just below the accuracy performance limit.

Time series of daily zonal mean ozone for Pacific Box



Time series of daily zonal mean ozone for Pacific Box for 2013



SDR Path Forward (Solution Key: DONE, READY, KNOWN APPROACH, UNKNOWN, *FUTURE WORK*)

A. OMPS NP Ozone Profile

A.i. Turn on the 253 nm channel in the retrieval algorithm -- DONE.

A.ii. First version of the stray light correction. – March 17 in Mx8.3 DONE.

A.iii. Improved/tuned stray light correction table -- April (SDR Table Tuning) Analysis shows more work is needed. Which channels are the best proxies?

A.iv. New Day 1 Solar irradiance spectrum and wavelength scale – May (SDR Table Tuning)
I recommend that this be a simple -0.115 nm shift relative to Day 0. We would revisit with annual wavelength scale variations and wavelength dependent shifts in the future. (Should this also adjust the radiometric coefficients for the shift/dichroic? Should the solar activity level be picked for the current Mg II 27-day average state?)

A.v. Proper matchup for Nadir Mapper and Nadir Profiler FOVs – TTO May 19 in Mx8.4 (EDR only).

A.vi. Error in smear subtraction creating offset bias error – Correct code (in Mx8.5), Change Input Bias to 742 counts.

A.vii. Soft Calibration adjustments including dichroic to Day 1 Solar or CF Earth -- May (SDR Table Tuning*).*

A.viii. Annual variations in the wavelength scale correlated with temperature gradients. SDR.

A.ix. Adjustments to Day 1 Solar for solar activity. SDR.

B. OMPS NM Total Column Ozone

B.i. Measurement-based wavelength scale adjustments – February 19 Mx8.1. DONE.

B.ii. Revised profile mixing fraction logic – March 17 in Mx8.3 (EDR only) DONE

B.iii. First version of OOR Table for the stray light correction -- May (SDR Table Tuning and Code Change)
New Table received. OOR cross-track dependence requires code change.
CCR to proceed with this for the Mx8.5 build. It is a change to the code and table dimensions. Minor ATBD and OAD and CDFCB changes.

B.iv. New Day 1 Solar irradiance spectra and wavelength scales. Should be set to middle of orbital scale variation. Cross-track dependence is complex. – May (SDR Table Tuning)

B.v. Soft Calibration adjustments to Day 1 Solar or CF Earth -- May (SDR Table Tuning)

B.vi. *Check flagging and logic for total ozone out of range and fill for triplet retrievals. (EDR)*

B.vii. *Possible bandpass changes -- ground to flight, intra-orbit.*

Lines of Code for V8TOz

- 1) To prepare LUT: 1252 lines
- 2) To generate files and prepare SDR and GEO for processing: 920 lines
- 3) The algorithm source codes: 19828 lines

Total lines: 22000 lines.

Options for Basic Implementation of V8TOz

- IDPS (Need to introduce new Process, LUTs and output)
  - Implement as a follow-on process to the MTTOz. Make use of the INCTO input/output as input. INCTO still run in IDPS, or
  - Replace MTTOz with V8TOz as PRO.
    - Minor changes to select 12 channels from the current 22, add/remove some input tables and output parameters.
- NDE
  - Implement as a new process
    - Transition V8TOz implementation for OMPS on LINUX in use at STAR. Only SDRs and GEOs continue in IDPS.
    - Need OMPS NM SDRs (SOMPS) and GEOs (GOTCO) delivered to the NDE system
- OSPO/POES
  - Implement as another "GOME-2" with existing V8TOz processing code
    - Reader in use at STAR can provide V8TOz with GEO and 12 channels. Only SDRs and GEOs continue in IDPS.
    - Need OMPS NM SDRs (SOMPS) and GEOs (GOTCO) delivered to the POES system

What about future refinements for V8TOz?

Path to upgrades

Information concentration

Information concentration can be performed at the same step as the N-value creation, either in the input stage of the MTTOz or the input stage of the V8TOz (if the latter is working from SDRs).

Additional channels for SO2 and NO2

These would be best implemented as stand-alone processes/products, although one of the SO2 options can work directly from the V8TOz residuals

Smaller FOVs

Under the current plan, these products would not flow from IDPS starting points for SDRs or EDRs as those would use an aggregator.

The bookkeeping for retrieving total ozone for smaller fields of view from an SDR is simple but the output products would have to be resized or be dynamically sized whether for the MTTOz or V8TOz.

New ancillary Input

IDPS can access better data for snow/ice and surface pressure and use these in the V8TOz processing

So can NDE and OSDPD

We have removed most of the dependencies on VIIRS and CrIS EDRs.

Options for Basic Implementation of V8Pro

- IDPS (Need to introduce new content and format for LUTs and output in addition to new PRO components)
  - Implement as a companion process to the V6Pro. Make use of the V6Pro input/output as input. V6Pro still runs in IDPS. (Tested in ADL at STAR.), or
  - Replace V6Pro with V8Pro as the Program part of IPO.
- NDE (Need to implement as a new process with new output)
  - From IMOPO – no new glueware, V6Pro still runs in IDPS, or
    - Need flow of IMOPO to NDE
  - From SONPS/GONPO & SOMTC/GOTCO – New glueware (in use at STAR), Only SDRs and GEOs in IDPS
    - Need flow of SDRs and GEOs to NDE
- OSPO/POES (Need to implement as another “SBUV/2” with existing V8 processing code)
  - From IMOPO – no new glueware, V6Pro still runs in IDPS, or
    - Need flow of IMOPO to POES processing system
  - From SONPS/GONPO & SOMTC/GOTCO – New glueware (in use at STAR), Only SDRs and GEOs in IDPS
    - Need flow of SDRs and GEOs to POES processing system

Lines of Code for V8Pro at STAR

- 1) To prepare LUT: 1253 lines
- 2) To generate orbit files, match up FOVs, and prepare SDRs and GEOs for processing: 1228 lines
- 3) Algorithm source codes: 15319 lines

Total lines: 17800 lines.

What about future refinements for V8Pro?

Solar Activity and Wavelength Scales in the SDR or when SDR is read in.

The daily Mg II Index values from GOME-2 can be used to adjust the Day 1 solar by using scale factors.

The day of year values can be used to give the expected wavelength scale from intra-annual variations. The can be used to adjust the Day 1 solar and its wavelength scale. (The V8Pro can accommodate small variations in the wavelength scale about some mean values.)

Information concentration / Noise reduction and Outlier Detection and Removal

Information concentration can be performed at the same step as the N-value creation, either in the input stage of the V6Pro or the input stage of the V8Pro (if the latter is working directly from SDRs). SONPO would maintain spectral coverage for smaller FOVs.

Smaller FOVs

Under the current plan, these products would not flow from IDPS starting points for SDRs or EDRs as those would use an aggregator.

Recommend that the “aggregator” have a “non-aggregator” switch and we develop smaller FOV capabilities as part of V8Pro implementation.

Glueware (NM/NP Matchups) modifications on the appropriate system would be needed to handle new cases of FOVs.

New ancillary Input

All three systems can access better data for snow/ice and surface pressure for use in the V8Pro processing

Recommendations for V8Pro

- OMPS ozone profile products should be made by using the V8Pro code as implemented for the SBUV/2.
  - This will require a flow of OMPS SDRs and GEOs.
  - Is this a long-term solution?
- The operational products should be the first step in CDR generation.
- Smaller FOVs should be accommodated by changes in the matchup glueware. Output products should be dynamically sized.
- Information concentration (noise reduction), outlier detection, solar activity adjustments, and intra-annual wavelength shifts should be implemented in the OMPS data input module for the V8Pro.
- Can the V8Pro in ADL jumpstart the IDPS.