Validated Stage 1 Science Maturity Review for OMPS Nadir Ozone Profile EDRs

Presented by L. Flynn, NOAA September 3, 2014

Outline

- Algorithm Cal/Val Team Members
- Product Requirements
- Evaluation of algorithm performance to specification requirements
 - Evaluation of the effect of required algorithm inputs
 - Quality flag analysis/validation
 - Error Budget
- Documentation
- Identification of Processing Environment
- Users & User Feedback
- Conclusion
- Path Forward

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
JAM	Maria Caponi	JPSS/Aerospace	Coordination, DRs, CCRs
Member	Bhaswar Sen	NGAS	Current Algorithms

Raytheon team members with major contributions include Derek Stuhmer and Daniel Cumpton.

Table 4.2.4 - Ozone Nadir Profile (OMPS-NP)			
Attribute	Threshold	Objective	
Ozone NP Applicable Conditions: 1.			
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 of along-track motion). The OMPS Nadir Pro OMPS Nadir Profiler performance is expected	cm cross-track by along -track FOV. It makes its offiler is designed to be operated in a mode that is ed to degrade in the area of the South Atlantic A	s 12 measurements over 24 Samples (160 km s able to subsample the required HCS. 2. The nomaly (SAA) due to the impact of periodic	

OMPS Nadir Profiler performance is expected to degrade in the area of the South Atlantic Anomaly (SAA) due to the impact of charged particle effects in this region. 3. All OMPS measurements require sunlight, so there is no coverage in polar night areas.

Data Product Maturity Definition

Validated Stage 1:

Using a limited set of samples, the algorithm output is shown to meet the threshold performance attributes identified in the JPSS Level 1 Requirements Supplement with the exception of the S-NPP Performance Exclusions.

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 eight shortest wavelengths (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 <u>474-00026</u> Rev-Baseline.pdf

OMPS NP OAD 474-00067 OAD-OMPS-NP-IP-SW RevA 201

Intermediate Product CDFCB

<u>474-00001-04-01 CDFCB-Vol4-Part1 Rev- Block-1-1 31Mar2011.pdf20127.pdf</u>

Nine Things to Know about the OMPS NP SDR

- System linearity is stable and well-corrected.
- Dark currents continue to trend higher but measurement signal-to-noise ratios remain high – weekly dark updates are flowing into the system and have good accuracy. The products are properly flagged in the SAA.
- Stray light corrections have been implemented and reduce this error significantly.
- An annual cycle of wavelength scale shifts has been identified. Causes, corrections and impacts have been investigated.
- A second round of Day 1 Solar spectra are in testing.
- Soft Calibration adjustments can be used to remove much of the bias with SBUV/2 results.
- Evidence of changes in the Dichroic throughput due to a ground-to-orbit shift are under investigation.
- The first year of solar measurements shows good long-term stability of instrument throughput and wavelength scales. There is some degradation at the shorter channels, e.g., 0.5%/year at 253 nm. Time-dependent (twice a year) Calibration Factor Earth values will be needed at some point in the future.
- Solar variability is not currently modeled in the SDR.
- KEY: Work needed to reach V1. Future work.

Evaluation of algorithm performance to specification requirements

- Findings/Issues from Provisional Review
 - SDR performance
 - Stray light errors present
 - Wavelength Scale (Annual Cycle)
 - Solar Activity (Mg II Index)
 - Absolute Calibration or radiance/irradiance ratios
 - EDR performance
 - 252 nm channel switched off
 - Snow/Ice not using the best data sets
 - Switched profile and total column error flags
- Improvements since Provisional
 - Algorithm Improvements
 - Stray light correction implemented (in SDR)
 - Smear/Bias error found and corrected (in SDR)
 - Corrected switched profile and total column error flags
 - Turned on 252 nm channel in retrieval February 2014
 - NM/NP mismatch found and corrected (in Glueware)
 - Calibration Table Updates in Progress
 - Continued weekly updates of Dark Tables
 - New Day 1 Solar and Wavelength Scale in testing
 - Awaiting new Day 1 solar results and Soft Calibration via Calibration Factor Earth (CFE) table

Evaluation of algorithm performance to specification requirements

- Findings/Issues in the last week
 - Glueware has hardcoded wavelengths that differ from the input parameters and RT LUT. Differences at the 13 channels are 1.54 0.13 -0.06 0.06 0.14 0.00 -0.08 -0.06 -0.01 0.00 0.05 -0.17 -0.18 nm. Differences in ozonecross sections (Alphas) are less than 1%.
- Cal/Val Activities for evaluating algorithm performance:
 - Comparisons to NOAA-18 and NOAA-19 SBUV/2
 - Zonal means (with SAA region removed)
 - Chasing orbits (Opportunistic Formation Flying OFF)
 - Comparisons include initial and final residuals (biases and standard deviations), ozone layer and ozone mixing ratio profiles, total ozone and reflectivity
 - www.star.nesdis.noaa.gov/icvs/prodDemos/index.php
 - Comparisons to Umkehr retrievals
 - Overpass data sets for NOAA network of Umkehr stations



Chasing orbit comparisons of SBUV/2 and OMPS-NP Version 6 Ozone Profiles for <u>July 10,</u> <u>2013</u>. Figures (a)-(I) 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.



Chasing orbit comparisons of SBUV/2 and OMPS-NP Version 6 Ozone Profiles for <u>May 23</u>, <u>2014.</u> Figures (a)-(I) show the 12 Umkehr layer amounts versus latitude for the two products. The layer lower boundaries are given in hPa above the figures. The two orbits are within 20 km and 15 minutes of each other at the Equator.



Chasing orbit comparisons of NOAA-19 SBUV/2 and OMPS-NP Version 6 results for July 10, 2013. Figures show channel initial measurement residuals versus latitude for the nine profiling wavelengths for the two products.



Chasing orbit comparisons of NOAA-19 SBUV/2 and OMPS-NP Version 6 results for May 23, 2014. Figures show channel initial measurement residuals versus latitude for the nine profiling wavelengths for the two products.

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 ΔXr computed directly and the * symbols are $Dy \Delta M$ with ΔM computed from the initial residuals.

See also <u>www.atmos-meas-tech.net/5/2951/2012/amt-5-2951-2012.html</u> DeLand, M. T., Taylor, S. L., Huang, L. K., and Fisher, B. L.: Calibration of the SBUV version 8.6 ozone data product, Atmos. Meas. Tech., 5, 2951-2967, doi:10.5194/amt-5-2951-2012, 2012.

Open DRs at or since Provisional

DR #	Short Description
7334	Impact of dichroic shifts (Use NP < 310 nm)
7335	Impact of time-dependent solar activity
7283	Use of Medium Resolution Data in Nadir Profile
7260	Impact of Annual wavelength scale shift cycle
7013	Activate 252 nm Channel (CCR Completed)
4802	Snow/Ice flag is 0 everywhere
4256	Improved Algorithm for OMPS Nadir Ozone Profile EDR
7623	Stray light correction (New, CCR completed)
7630	Incorrect spatial pixel for bias calculation (New, CCR completed) ¹⁷

Open DRs Today

DR #	Short Description
7334	Impact of dichroic shifts (SDR stable; Soft Calibration 5074)
7335	Impact of solar activity (SDR small; endure, future)
7283	Use of Medium Resolution Data in Nadir Profile (Future; J1)
7260	Impact of wavelength scale shift (Small after 7450; endure)
4802	Snow/Ice flag is 0 everywhere (Small; endure for Val Stage1)
4256	V8 Algorithm for Profile EDR (Future)
7654	Day 1 Solar Spectra (SDR Update in testing)
7450	Day 1 Wavelength Scale (SDR Update to annual average in testing; endure 7260)
5074	Generate soft calibration coefficients (Set SDR CFE using initial residuals and chasing orbits from NOAA-18/19 SBUV/2; time-dependent CFE for future degradation.)
NEW ####	Incorrect wavelengths hardcoded in glueware. (SDR small after 5074; endure until CCR for Mx8.8)

Evaluation of the effects of marginal algorithm corrections

- Desired Algorithm Improvements in SDR
 - Better Stray Light correction
 - Annual cycle of Wavelength Scales
 - Variations for Solar Activity
 - Time-dependent Instrument Degradation
 - Outlier detection / information concentration
- Evaluation of the effect of marginal algorithm inputs
 - Error Bounds and Sensitivity Analyses

Analysis of Solar Measurements for the Working Diffuser



Spectral Patterns and Their Temporal Coefficients



Diffuser and Instrument Degradation

Working & Reference Trends



22

Variations (Maximum minus Minimum) in shorter wavelength channels from linear fit with 299 nm variations. May 15, 2013 vs. May 16, 2014



The solid line shows the range of variations relative to polynomial fits of Earth radiances for low SZA cases that are correlated with similar variations for the 299 nm wavelength channel. The solid line shows the behavior before applying a laboratory-based stray light correction and the dotted line shows the behavior with the correction applied. The correction reduces the stray light by over 50% and the errors are now within limits. The vertical red lines are retrieval channel locations.



Upper Left Umkehr Layer 12 and above (> 0.25 hPa)Upper Right Umkehr Layer 11 (0.5 - 0.25 hPa)Lower Left Umkehr Layer 10 (1.0 - 0.5 hPa)Lower Right Umkehr Layer 9 (2.0 - 1.0 hPa)Without corrections, stray light contributes to both the accuracy and precisionerror budgets for the upper layers.

Scatter Plots of Ozone Layer Variations versus Reflectivity VariationsReduced strayfor the first five orbits of May 16, 2014



Scatter gives an upper limit on effect of instrument noise on the retrieval precision as there are real variations for different orbits and latitudes.

Instrument Performance

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	< 0.01 nm #
Stray Light NM Out-of-Band + Out-of-Field Response	≤ 2%	average ~± 1%*
Intra-Orbit Wavelength Stability	<0.02 nm	< 0.01 nm
SNR	Channel Dependent	As good as SBUV/2 at Alg. Channels &
Inter-Orbital Thermal Wavelength Shift	<0.02 nm	0.03-nm amplitude 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%

- # After new analysis of Day 1 Solar
- * After measurement-based correction using prelaunch characterization
- ^ Regular annual cycle affects accuracy and stability
- & Information concentration possible by using near-by channels.

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

 New DR####: Small (1% in alpha) error from incorrect channel assignment in glueware. Will be removed to first order with soft calibration as it is primarily a bias.

Quality flag analysis/validation

- Quality Flags
 - Switched names corrected. (July 2013)
 - SAA Functioning properly.
 - Ascending/Descending fixed (August 2013).
 - Terrain pressure limit fixed (February 2013)
 - No snow ice reported.
- Other quality flag analysis/validation Provided in Provisional report. Summary on the next slide.

IMOPO Error Flags

- Individual Flags
 - Sun Glint, SAA, and Eclipse are all set correctly
 - SO2 Index is running too negative; it and the Volcano Contamination Index (VMI) are affected by initial calibration uncertainties.
 - Snow/Ice is always zero DR #4802
- Profile Error Codes*
 - Code 1 is set correctly (Lower three layers)
 - Code 2 is set correctly (BestTOZ vs ProTOZ)
 - Code 3 is set correctly (large final residuals often for data in SAA)
 - Code 5 is set correctly (C outside of range often for data in SAA)
 - Codes 4, 6, 7 & 8 conditions are not met in samples
 - Code 9 (Bad counts/missing measurements)
 - Code 20 Invalid or out-of-range inputs Flagged all terrain pressure > 1.001 atm. until fixed in February 2013.
 - Descending Flag (+10) in error, fixed with DR 5046/CCR881 in Mx8.0.
- Total Ozone Error Codes*
 - Codes 1 & 2 are set correctly by comparing S x Omega to 1.5 and 3.5 atm-cm, respectively
 - Code 4 is set correctly (Pair differences)
 - TOZ Error Code 5 matches PRO Code 2
 - Code 7 not seen; Photometer Reflectivity difference is not in the output. All channels are coincident.
 - Codes 8 & 9 conditions are not met in samples; Codes 3 & 6 are Spares
 - Code 20 Invalid or out-of-range inputs matches profile behavior
 - Descending Flag (+10) matches Profile Error behavior
- *Profile and total ozone error flags were switched in the HDF5 output. This was fixed with the implementation of PCR 27740 in 2013.

Documentation

• The following documents will be checked to ensure consistency with current codes and performance, updated as needed, and provided to the EDR Review Board before AERB approval:

– ATBD

- 474-00026 (April 2011) Joint Polar Satellite System (JPSS) OMPS Nadir Profile Ozone Algorithm Theoretical Basis Document (ATBD)
 - OAD
- 474-00067 Revision C: Joint Polar Satellite System (JPSS) Operational Algorithm Description (OAD) Document for Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Intermediate Product (IP) Software
- 474-00448-03-22 Joint Polar Satellite System (JPSS) Algorithm Specification Volume III: Operational Algorithm Description (OAD) for the Ozone Nadir Profile EDR
 - Updated README file for CLASS
- Revising Provisional Release Readme.
- Algorithm References:
 - Version 6: Bhartia, P. K., McPeters, R. D., Mateer, C. L., Flynn, L. E., and Wellemeyer, C.: Algorithm for the estimation of vertical ozone profiles from the backscattered ultraviolet technique, J. Geophys. Res.-Atmos., 101, 18793–18806, 1996.
 - Version 5: <u>http://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/19900007911.pdf</u>
 - Version 8: Bhartia, P. K., McPeters, R. D., Flynn, L. E., Taylor, S., Kramrova, N. A., Frith, S., Fisher, B., and DeLand, M.: Solar Backscatter UV (SBUV) total ozone and profile algorithm, Atmos. Meas. Tech. Discuss., 5, 5913\u20135951, doi:10.5194/amtd-5-5913-2012, 2012.

Identification of Processing Environment

- IDPS Mx8.6 (With planned revision for Mx8.8 February 2015)
- Algorithm version (Version 6 SBUV algorithm) as adapted for OMPS with additional CCRs.
- IDPS Build: I1.05.08.05 (Mx 8.5)
- EDR version: Mx 8.5
- LUT Version: PS-1-O-CCR-13-0829-JPSS-DPA-002-PE
- PCT Version: N/A
- Environment for testing: Linux (ADL Mx 8.x) and AIX (ADA Mx 8.x)

Users & User Feedback

- Users list
 - NCEP, NASA, NRL, Environment Canada, EuMetSat
- Feedback from users
 - BUFR product in testing at NCEP, EC, and EuMetSat
- Downstream product/application list
 - NCEP assimilation (UV Index and weather)
 - Ozone Hole Monitoring (Six-month Stratospheric Summaries)
 - Ozone Layer Assessments
 - TOAST daily ozone maps
- Reports from downstream product teams on the dependencies and impacts
 - Calibration bias creates offsets with NOAA-19 SBUV/2 products
 - Desire for averaging kernels in BUFR product (with V8Pro)



OMPS SH



Monthly Mean Ozone Mixing Ratio Differences : July 2014 Comparison with N19 SBUV/2



Conclusion

- Cal/Val results summary:
 - Team recommends product advancement to Validated Stage 1 Maturity effective with key corrections
 - CCRs for three SDR DRs (All to Tables not to Code)
 - DR 7654 OMPS NP SDR Nadir Profiler Day 1 solar irradiance spectrum update
 - DR 7450 OMPS NP SDR OMPS NP Wavelength Scale
 - DR 5047 OMPS NP IP Generation of soft calibration coefficients for NP IP – Use chasing orbits and calibrate to NOAA-19 SBUV/2
 - CCR to change hard-coded wavelengths in Glueware.

Path Forward

- Areas with planned further improvements
 - Information concentration / outlier detection
 - Implement V8Pro algorithm and Small FOV
 - Model solar activity
 - Snow/Ice use daily forecast tilings
 - Implement annually varying wavelength scale
- Planned Cal/Val activities / milestones
 - December 2014 Show improved comparisons to NOAA-19 SBUV/2 and ground-based Umkehr with new SDR.
 - March 2015 extend analysis to show Validated Stage 2.
 - July 2015 demonstrate stability and annual cycle analysis to show Validated Stage 3.

Backup

Initial Measurement Residuals for OMPS-NP and SBUV/2 Version 6 Algorithm

Weekly Dark Updates Began



Requirements (1 slide)

Product Requirements from JPSS L1RD

Attribute	Threshold	Objective
Geographic coverage		
Vertical Coverage		
Vertical Cell Size		
Horizontal Cell Size		
Mapping Uncertainty		
Measurement Range		
Measurement Accuracy		
Measurement Precision		
Measurement Uncertainty		

Error Budget

Compare analysis/validation results against requirements, present as a table. Error budget limitations should be explained. Describe prospects for overcoming error budget limitations with future improvement of the algorithm, test data, and error analysis methodology.

Attribute Analyzed	L1RD Threshold	Analysis/Validation Result	Error Summary

State of the Ozone Profile Product

- The OMPS Nadir Profile product is created by using the Version 6 SBUV/2 algorithm.
- The product is currently at provisional status awaiting new Day 1 solar spectra and wavelength scales and soft calibration adjustments to force it to agree with the NOAA-19 ozone profile products. These should be in place by the end of the year.
- An upgrade of the algorithm to the Version 8 SBUV/2 algorithm is progressing through testing and should be in operations by early next year.