Validated Maturity Science Review For NOAA-21 V8TOz & V8TOS Total Column Ozone EDR

Presented by L. Flynn Date: 09/19/2024

https://drive.google.com/drive/u/0/folders/1y6wbuhxNp3Jcbevfh9GICmJ8LtP9iSPV

Disclaimer:

"The scientific results and conclusions, as well as any views or opinions expressed herein, are those of the authors and do not necessarily reflect those of NOAA or the Department of Commerce."



1. <u>Beta</u>

- Product is minimally validated, and may still contain significant identified and unidentified errors.
- Information/data from validation efforts can be used to make initial qualitative or very limited quantitative assessments regarding product fitness-forpurpose.
- o Documentation of product performance and identified product performance anomalies, including recommended remediation strategies, exists.

2. <u>Provisional</u>

- Product performance has been demonstrated through analysis of a large, but still limited (i.e., not necessarily globally or seasonally representative) number of independent measurements obtained from selected locations, time periods, or field campaign efforts.
- o Product analyses are sufficient for qualitative, and limited quantitative, determination of product fitness-for-purpose.
- Documentation of product performance, testing involving product fixes, identified product performance anomalies, including recommended remediation strategies, exists.
- Product is recommended for potential operational use (user decision) and in scientific publications after consulting product status documents.

3. Validated

- Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).
- Comprehensive documentation of product performance exists that includes all known product anomalies and their recommended remediation strategies for a full range of retrieval conditions and severity level.
- Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.
- \circ $\,$ Product is ready for operational use based on documented validation findings and user feedback.
- o Product validation, quality assurance, and algorithm stewardship continue through the lifetime of the instrument.



- Product Requirements
- Pre-launch EDR Performance Matrix/Waivers None
- Validated Maturity Performance Validation
 - On-orbit instrument performance assessment
 - Identify all of the instrument and product characteristics you have verified/validated as individual bullets
 - Identify pre-launch concerns/waivers, mitigation and evaluation attempts with on-orbit data
- Users/Downstream Products EDR feedback
- Risks, Actions, Mitigations
 - Potential issues, concerns
- Path forward
- Summary

Past EDR Concerns for OMPS NM SDRs

- Latitude dependence of differences between NPP, N20 and N21 for V8TOz after equatorial adjustments to force agreement. Greatly reduced for latest results.
- Inclusion of OOBR stray light correction for N21 OMPS NM New correction table in use.
- Solar Spatial discontinuities for N21 OMPS NM Handled by soft calibration.
- Solar bias versus reference spectra for N21 OMPS NM Handled by new Day 1 solar calibration.
- Solar updates for degradation Not yet a concern for NOAA-21 OMPS NM.



- Algorithm Cal/Val Team Members
- Product Overview/Requirements
- Evaluation of algorithm performance to specification requirements
 - Algorithm version, processing environment
 - V8TOS Performance and Improvement
 - Evaluation of the effect of required algorithm inputs
 - Soft Calibration Adjustments
 - Quality flag analysis/validation
 - Error Budget
- User Feedback
- Downstream Product Feedback
- Risks, Actions, and Mitigations
- Documentation (Science Maturity Check List)
- Conclusion
- Path Forward



Ozone Cal/Val/Alg Team Membership

EDR	Name	Organization	Task
Lead	Lawrence Flynn	NOAA/NESDIS/STAR	Ozone EDR Team
Sub-Lead	Irina Petropavlovskikh	NOAA/ESRL/CIRES	Ground-based Validation
Sub-Lead	Trevor Beck	NOAA/NESDIS/STAR	Trace Gas Algorithm Development
Member	Jianguo Niu	STAR/IMSG^	R&D, trouble shooting, TOAST, V8TOS
Member	Eric Beach	STAR/IMSG^	Validation, ICVS/Monitoring, Data Management
Member	Zhihua Zhang	STAR/IMSG^	V8 Algorithms implementation & modification
Member	Robert Lindsay	STAR/IMSG^	Limb Algorithms implementation
Member	Jeannette Wild	UMD	Applications, CDRs, validation
JAM	Starry Manoharan	JPSS/KBR	Coordination
Adjunct	Bigyani Das	STAR/ASSISTT	Deliveries to NDE / NCCF
PAL	Vaishali Kapoor	OSPO	Atmospheric Chemistry Product Area Lead
SDR	Banghua Yan	NOAA/NESDIS/STAR	OMPS SDR Lead



Product Overview/Requirements

 Product performance requirements from JPSS L1RD supplement (threshold) versus observed/validated/JERD Vol. II

Attribute	Threshold	Observed/Validated	
Geographic coverage	90% Daily Global Earth	SZA < 80° (>90% coverage)	
Vertical Coverage	0-60 km	0-60 km (RT tables, physics)	
Vertical Cell Size	NA	NA	
Horizontal Cell Size	50x50 km ² at nadir	10x9 km ² at nadir	
Mapping Uncertainty	5 km at nadir	3 km at nadir (SDR Team)	
Measurement Range	50 – 650 DU	90-700 DU (algorithm performance and real range)	
Measurement Accuracy			
X < 250 DU	9.5 DU	6.0 DU^	
250 DU < X < 450 DU	13.0 DU	10.0 DU^	
X > 450 DU	16.0 DU	12.0 DU^	
Measurement Precision	for 50x50 km ² product	for 10x9 km ² product (Broadband)	
X < 250 DU	6.0 DU	1 DU* +0.5%	
250 DU < X < 450 DU	7.7 DU	1 DU* +0.5%	
X > 450 DU	2.8 DU + 1.1%	1 DU* +0.5%	

^within ±0.5%VersusS-NPP & NOAA-20V8TOz for latitudebands

*SDR contribution from Double-Centered Difference + Dark Updates



- Findings/Issues from Provisional Review
- Improvements since Provisional Review
 - Algorithm Improvements
 - LUT / PCT updates
- Algorithm performance evaluation
 - Validation data sets (type, periods, coverage)
 - Validation strategies / methods
 - Validation results
 - Long term monitoring readiness
- Inter-sensor comparison
 - Compare with S-NPP and NOAA-20
 - Compare with other satellite product



OMPS NM SDR Changes since Provisional Review

ADR	CCR	Title	Description	Build	Status
10360	6548	Fixing Straylight deficiency in N21 OMPS NM	The OMPS NM SDR data quality show a strong latitude dependency at short wavelengths. This problem gradually increase the inter-sensor radiance biases at short wavelengths. The root cause is from SL table being initialized at N20 NM cross-track resolution (35 pixels) instead of N21 NM resolution (177 pixels).	Mx8	In Operation 6/23/2023
10365	NA (Fast Track)	Investigate 0.03 nm difference in EV and Solar Irradiance wavelength scale	Use the solar Mg-II 280nm absorption feature. This method is consistent with the earth view radiance approach and the SNPP and NOAA-20 solar approaches. Updated via weekly fast track updates.		In Operation 11/06/2023
10553	6799	OMPS-NP Hot pixel/ Transient Pixel	One single CCD pixel began to exhibit unstable dark current background signal several months in to the mission. A flight table and ground table updates effectively disabled the transient pixel.	MX8	In Operation 01/26/2024
10550	6767	Solar intrusion OMPS NP straylight correction	The preliminary analysis of NOAA-21 OMPS shows solar intrusion in the NP radiance. This straylight effect needs to be corrected.	Mx8	In Operation 11/09/2023
10552	6773	Solar Intrusion for OMPS NP – code change	This stray-light effect needs to be corrected across NOAA-21, NOAA-20, and SNPP. This requires code change.	Mx10	TTO 5/16/2024
	NA (Fast track)	OMPS NP Dark Overcorrection	Updated via weekly fast track updates.		In Operation
10685	6951	N21 OMPS NP Straylight Correction	Performance of NOAA-21 OMPS NP straylight LUT currently used in IDPS operations is not optimal and needs improvement for better calibrated SDR that leads to higher quality EDR products.	Mx9	In Operation 03/01/2024
10686	6956	N21 OMPS NM out-of-band straylight correction	This stray light calibration table is to correct stray light effects from wavelengths above 380nm on short wavelengths for NOAA-21 OMPS NM SDR data.	Mx9	In Operations on 03/21/2024
10825	7105	Assess calibration errors in NOAA-21 OMPS NM and NP solar flux relative to S-NPP	The solar flux differences in NOAA-21 OMPS NM and NP have been identified by comparing S-NPP day-1 and synthetic spectra	Mx9	In Operations on 04/11/2024
10832	TBD	Correcting instruments degradation and solar activity impacts in OMPS biweekly solar tables.	There are two parts: The 1 st is the solar activity correction which will be updated and delivered as the biweekly solar fast track LUTs for all the three sensors (NPP, N20 and N21). The 2 nd involves calibration factor update.	MX10	Target: Oct. 2024

OMPS NM SDR Changes or Findings since SDR Provisional

- The OMPS NM Solar Irradiance Spectra were adjusted to 1 AU.
 - This created a change of ~2.5% in the radiance / irradiance ratios.
- The Solar Irradiance Spectra were adjusted by ~-3% to improve the absolute calibration
- The OMPS NM SDR Straylight correction was too small by a factor of ~10.
 - This produces a latitude-dependent (SZA, SVA, reflectivity and ozone dependent) bias in the radiances. The bias in the radiances may be partially responsible for a latitude-dependent bias in the total ozone of 2% seen at Beta & Provisional Maturity.
 - The improved straylight correction (in operations since June 26, 2023) changes the biases in the tropics where the V8TOz soft calibration adjustments are developed.



- Description of processing environment and algorithms used to achieve the maturity stage:
 - Algorithm version: STAR Offline V8TOz v4r5 NCCF V8TOz v4r4 \rightarrow v4r5 with latest delivery
 - Version of LUTs used: Second Instrument Radiative Transfer Tables 09/10/2024
 Third Soft Calibration Adjustment Table 09/10/2024
 - Effective date: TBD 10/xx/2024



- Required Algorithm Inputs
 - OMPS Nadir Mapper SDRs and Geos
 - Instrument Radiative Transfer Tables
 - Soft Calibration Adjustment Tables
- Change to error handling in V8TOS algorithm for all three satellites.
- No changes to the V8TOz EDR algorithm Table updates only.
 - Revised instrument radiative transfer table 04/15/2023
 - Soft Calibration Adjustment Table #1 05/10/2023
 - Soft Calibration Adjustment Table #2 August 2023
 - Soft Calibration Adjustment Table #3 September 2024
 - Revised instrument radiative transfer tables #2 September 2024



NOAA-20 NM Daily Wavelength Scale on 2023/03/13

Updated at Mar 14 16:52:10 2023 UTC

NOAA-21 OMPS NM has a smaller intraorbital wavelength scale variation than NOAA-20 OMPS NM. Both are wellcharacterized by the granule-level adjustments in the SDR processing, the adjustments are good.



Smaller FOV have noisier measurements as expected





V8TOS Performance for NOAA-21





V8TOS Performance for NOAA-20





Before and After Maps for N21 V8TOS Flag Identification Upgrade





The increased noise in the NOAA-21 SO2 estimates is expected. We are investigating methods to use local fits (wavelength channel intervals) of radiance / irradiance rations to identify outliers and filter the measurements to reduce the noise.

The two earlier slides showed the good performance for a recent volcanic event in Russia.



Soft Calibration Approach

The purpose of generating Soft-Calibration Adjustments for N21 V8TOz is to make its retrievals close to those from current operational S-NPP/NOAA-20 V8TOz.

16 consecutive days' (Mar14-29, 2024) of data that have full daily orbits with stable SDR were selected to create adjustments.

Note: Dates around the Equinoxes – Mar. 21 or Sep. 21 – are better for generating high quality soft-calibration.

Z. Zhang, et al., An Approach to Track Instrument Calibration and Produce Consistent Products with the Version-8 Total Column Ozone Algorithm (V8TOz)



NOAA-21 Calibration/Validation Maturity Review



NOAA-21 Calibration/Validation Maturity Review





Cross-track dependence of Ozone, Aerosol and 1-percentile Reflectivity over the Equatorial Pacific before and after soft calibration compared to S-NPP and NOAA-20.







One day's (3/17/2024) retrievals with the new soft-calibration for N21 V8TOz: Ozone Top Left, Aerosol Index Top Right, Effective Reflectivity Bottom Left.







One day's (3/17/2024) retrievals with the new soft-calibration for NPP V8TOz: Ozone Top Left, Aerosol Index Top Right, Effective Reflectivity Bottom Left.





One day's (3/17/2024) retrievals with the new soft-calibration for N20 V8TOz: Ozone Top Left, Aerosol Index Top Right, Effective Reflectivity Bottom Left.



















- Defined Quality Flags
 - Variable
 - Description
 - Value
- Quality flag analysis/validation
 - Test / example / ground truth data sets
 - Analysis / validation results
 - Analysis / validation plan



Quality Flags V8TOz Error Codes

Output	Name	Description
Error Flag	Good – 0	Good retrieval SZA <= 84°
	Sun Glint Geometry – 1	Good retrieval, open water with sun glint geometry present
	High SZA – 2	Good retrieval SZA > 84°
	Large Aerosol Index – 3	360 nm residual > threshold
	Profile Shape Error – 4	Residual at unused ozone wavelength > 4 σ Use with caution
	High SO ₂ – 5	SO_2 Index > 4 σ Use with caution
	Non-Convergence – 6	Algorithm does not converge
	Large Residual – 7	Absolute residual > 32
	Bad Radiances – 8	Negative or missing radiances (Partial Granule Fix)
Eclipse Flag	0 – Good, 1 – Eclipse	Solar Eclipse Condition










NOAA21 OMPS TC Radiance mW m⁻² nm⁻¹ sr⁻¹ 2023/04/20 at 331.1nm



NOAA21 OMPS NP Radiance mW m⁻² nm⁻¹ sr⁻¹ 2023/04/20 at 253.4nm



Solar Eclipse Flag for April 20, 2023



NOAA-21 OMPS TC Solar Eclipse Flag 2023/04/20

NOAA-21 OMPS NP Solar Eclipse Flag 2023/04/20





Comparisons of NPP Overpass to Dobson Stations, Boulder CO





Comparisons of NPP Overpass to Dobson Stations, Mauna Loa HI



NOAA-21 Calibration/Validation Maturity Review



Comparisons of NPP Overpass to Dobson Stations, Lauder NZ





Comparisons of NPP Overpass to Dobson Stations, Boulder CO







Comparisons of NPP Overpass to Mauna Loa, Hawaii



Month / Day in 2024



Comparisons of NPP Overpass to Haute Provence, France



NOAA-21 Calibration/Validation Maturity Review



Comparisons of NPP Overpass to Lauder, New Zealand



NASA NPP/OMPS Parameters



 Provide updates for the status of the risks/actions identified during the previous maturity review(s); add new ones as needed

Identified Risk	Description	Impact	Action/Mitigation and Schedule
Latitude Dependence	NOAA-21 V8TOz Zonal Means show 1-3% biases at higher latitudes versus NPP and N20.		Revise Stray Light OOR/B corrections; examine Polarization sensitivity.
Increased Noise	Smaller FOVs use less aggregation so measurements are noisier.	Error flags in SAA and at high SZA.	Develop and implement filtering / information concentration similar to that used for the V8Pro.
V8TOS Error Handling	V8TOS does not filter bad residuals as well as it should.	Creates bad values in retrievals	Provide revised code with improved filtering prior to Validated Maturity.



Science Maturity Check List	Yes
ReadMe for Data Product Users	Yes (after approval)
Algorithm Theoretical Basis Document (ATBD)	Yes
Algorithm Calibration/Validation Plan	Yes
(External/Internal) Users Manual	Yes
System Maintenance Manual (for ESPC products)	Yes
Peer Reviewed Publications (Demonstrates algorithm is independently reviewed)	Yes
Regular Validation Reports (at least annually) (Demonstrates long-term performance of the algorithm)	



Conclusions, Caveats and Path Forward at Provisional

- The NOAA-21 OMPS NM SDRs have improved performance as of the end of J 2023.
 - The OMPS NM SDRs have a corrected sample table update for macro-pixel #177.
 - The OMPS NM SDRs have 1-AU Day 1 solar irradiance.
 - The OMPS NM SDRs have a new stray light correction.
- While the NDE I&T NOAA-21 V8TOz and V8TOS v4r2 EDRs are reasonable
 - A 2nd iteration of soft calibration adjustments to force agreement with S-NPP and NOAA-20 V8TOz EDRs has been completed using data from July 2023. The table will be delivered in August 2023.
 - The smaller FOV measurements show increased noise especially in the SAA and for SO2 retrievals. We are developing outlier detection and local fitting processes to increase the SNRs of the values used in the retrieval algorithm. We will also be checking how well aggregation / averaging of the smaller FOVs recovers the performance obtained for NOAA-20.
 - A mishandling of bad values in the V8TOS during the background bias estimation step is leading to some errors in the SO2 values. We will provide a correction involving a modest amount of code changes this month.
 - We recommend that the NOAA-21 V8TOz & V8TOS EDRs from NDE I&T & NCCF be reported at Provisional Maturity as of implementation of the latest adjustment table. The product performance is very good for latitudes <u>within 35° of the Equator.</u> The OMPS V8TOz is in regular operations.



Validated Maturity End State	Assessment
Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).	Over one year of comparisons to ground-based and other satellites with progressively improving product.
Comprehensive documentation of product performance exists that includes all known product anomalies and their recommended remediation strategies for a full range of retrieval conditions and severity level.	This presentation covers the know anomalies – smaller FOV performance leads to noisy measurements resulting in noisier SO2 estimates and more error code 4 and 5 values.
Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.	Between test processing with new tables and regular processing with old tables, products are well-studied.
Products are ready for operational use based on documented validation findings and user feedback.	Total ozone products are ready for assimilation and trend studies. Aerosol Index and Reflectivity products are consistent with validated NPP and N20 products. SO2 products are ready for generating alerts.
Product validation, quality assurance, and algorithm stewardship continue through the lifetime of the instrument.	Monitoring and validation processes are on-going and regularly updated.

Conclusions, Caveats and Path Forward at Validated Maturity

- The NOAA-21 OMPS NM SDRs have improved performance as of the end of April 2024:
 - The OMPS NM SDRs have a new Day 1 Solar corrected for estimated biases.
 - The OMPS NM SDRs have a new stray light correction.
- The NCCF NOAA-21 V8TOz and V8TOS v4r5 EDRs are ready for operational use:
 - A 3rd iteration of soft calibration adjustments to force agreement with S-NPP and NOAA-20 V8TOz EDRs has been completed using data from March 2024. The table should be in use by October 2024.**
 - A revised set of instrument tables (RT and dN/dx) has been delivered. The tables should also be in use by October 2024.**
 - The smaller FOV measurements show increased noise compared to NPP and N20 especially in the SAA and for SO2 retrievals. Performance can be recovered by averaging.
 - We recommend that the NCCF NOAA-21 V8TOz & V8TOS v4r5 EDRs from NCCF be reported at Validated Maturity as of implementation of the latest adjustment table.





NASA estimates of the spectral dependence of the straylight components for OMPS NM SDRs







N20 changes without versus with NOAA straylight correction.



Additional Percent Change in Correction from OOB/R Straylight for a Flat Field







Old Bad RT Instrument Table





NOAA-20 RESULTS









Old Bad RT Instrument Table



New Good N21 RT Instrument Table



NOAA-20 RESULTS
















Zonal Mean Ozone Differences to NOAA NPP



Percentage





Comparison of Cross-track Retrieval Averages (STAR) NEW RT TABLE





Smaller FOVs show increased flagging in the SAA





Comparisons of UV-Absorbing-Aerosol Index estimates for February 17, 2023 from NOAA-20 OMPS (left) and NOAA-21 OMPS (right) showing African biomass burning features.



Comparisons of UV Absorbing Aerosol Index estimates from NOAA-20 OMPS (left) and NOAA-21 OMPS (right) for one day showing Saharan Dust (upper feature) and biomass burning (lower).



While the NOAA-21 product shows cross-track calibration biases in the initial calibration, the much improved spatial resolution with the small Fields-of-View is obvious.

3.42

4.50

2.33

-0.92

0.17

1.25

-2.00

-0.92

-2.00

0.17

1.25

2.33

3.42

4.50