Provisional Maturity Science Review For V8TOz & V8TOS Total Column Ozone EDR

Presented by L. Flynn Date: 08/03/2023



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. Provisional

- 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.
- 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.
- 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
- Provisional 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 feedback
- Risks, Actions, Mitigations
 - Potential issues, concerns
- Path forward (to the next maturity stage)
- Summary



- Provisional Maturity Performance is well characterized and meets/exceeds the requirements:
 - On-orbit instrument performance assessment
 - Provide summary for each identified instrument and product characteristic you have validated/verified as part of the entry criteria
 - Provide summary of pre-launch concerns/waivers mitigations/evaluation and address whether any of them are still a concern that raises any risk.
- Updated Maturity Review Slide Package addressing review committee's comments for:
 - Cal/Val Plan and Schedules
 - Product Requirements
 - {Beta/Provisional/Validated} Maturity Performance
 - Risks, Actions, Mitigations
 - Path forward (to the next maturity stage)



OMPS Ozone Provisional for V8TOz and V8TOS EDRs

https://drive.google.com/drive/u/0/folders/1uePzfr2LR9Bypy7Z6S0qNUcEa38VQE8q



- 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/Aerospace	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



OMPS TC EDR Performance Characteristics

	Threshold	Objective
Ozone TC Applicable Conditions 1, 2.		
a. Horizontal Cell Size	50 x 50 km^2 @ nadir	10 x 10 km^2
b. Vertical Cell Size	0 - 60 km	0 - 60 km
c. Mapping Uncertainty, 1 Sigma	5 km at Nadir	5 km
d. Measurement Range	50 - 650 milli-atm-cm	50-650 milli-atm-cm
e. Measurement Precision		
1. X < 0.25 atm-cm	6.0 milli-atm-cm	1.0 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	7.7 milli-atm-cm	1.0 milli-atm-cm
3. X > 0.45 atm-cm	2.8 milli-atm-cm + 1.1%	1.0 milli-atm-cm
f. Measurement Accuracy		
1. X < 0.25 atm-cm	9.5 milli-atm-cm	5.0 milli-atm-cm
2. 0.25 < X < 0.45 atm-cm	13.0 milli-atm-cm	5.0 milli-atm-cm
3. X > 0.45 atm-cm	16.0 milli-atm-cm	5.0 milli-atm-cm
g. Latency	90 min.	15 min.
h. Refresh	At least 90% coverage of	24 hrs.
	the globe Every 24 hours	
	(monthly average)	
i. Long-term Stability	1% over 7 years	0.5 % over 7 years
1. Threshold requirements only apply under daytime conditions with Solar Zenith	1 milli-atm-cm = 1 DU	
Angles (SZA) up to 80 degrees.		
2. The EDR shall be delivered for all SZA.		
3. SO2 exclusion removed.		



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	ent Precisionfor 50x50 km² productfor 10x9 km² product (Broad		
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%	

<u>^Versus NPP V8TOz</u>
for latitude bands

*SDR contribution from Double-Double Difference

+ Straylight Error



- Findings/Issues from Beta Review
- Improvements since Beta 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



- SDR
 - Stray Light Update but no OOB on June 26, 2023.
 - Solar and wavelength shift reviewed and 1 AU adjustment
 - Second N21 Reference diffuser solar measurement planned for August 25, 2023
 - Intra-orbit wavelength scale changes (smaller than NPP or N20).
 - Precision for SDR and EDR.
- Soft Calibration PRNU and absolute accuracy
 - Before / after Ref, AI, Ozone with soft calibration adjustments.
 - Maps of all three and error codes
- Latitude Dependence of Zonal means changed but still present
- V8TOS
 - Good for correcting for volcanic events.
 - New code needed for error flag handing.
- Comparison of NPP to Dobson stations
 - https://gml.noaa.gov/ozwv/dobson/plots/index.php?sta=ldr
- Smaller FOV considerations. Recover SNR?



- Description of processing environment and algorithms used to achieve the maturity stage:
 - Algorithm version:

– Version of LUTs used:

Effective date:

NDE I&T V8TOz v4r2 STAR Offline V8TOz v4r3 NCCF V8TOz v4r3 Revised instrument radiative transfer table 04/15/2023 Soft Calibration Adjustment Table 05/10/2023 Second Soft Calibration Adjustment Table 8/XX/2023 8/XX/2023, As the SDR matures, new adjustment tables will be

devised and delivered.



- Required Algorithm Inputs
 - OMPS Nadir Mapper SDR and GEO
 - Instrument Radiative Transfer Tables
 - Soft Calibration Adjustment Tables
- No changes yet to the V8TOz or V8TOS EDR algorithms 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 Delivery



Table A summary of the delivered and upcoming NOAA-21 OMPS NM and NP SDR LUTs as of 04/25/2023

#Delivery	Date of Used Working Diffuser Solar Data	Delivered LUTs	Affected Sensor	Main Purpose	Operational Date
1st	02/09/2023	OSOL and Wavelength LUTs (NM: - 0.13nm; NP: - 0.09nm)	NM and NP	Wavelength shifts from ground to flight; Fixing the NM radiance 3- pixel-shift- error	03/09/2023
2nd	03/19/2023	OSOL and wavelength LUTs	NP	Fixing the NP 12-pixel- error; wavelength shift since 02/09/2023	03/23/2023
3rd	02/09/2023	Sample table, OSOL and wavelength LUTs	NM	Fixing the 85 th cross- track wavelength shift discrepancy	04/13/2023
4th	04/16/2023	OSOL and wavelength LUTs	NP	Applied SED correction; doppler shift correction; wavelength shift	04/20/2023
5rd	Target: 04/27/2023 to ASSISTT	OSOL LUT	NM	Applied SED correction;	Target: 05/04/2023

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 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 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.



- Regular weekly dark table and biweekly Solar and wavelength table updates for both SDRs. The dual diffuser system is working well.
- Solar and wavelength updates for ground-to-orbit wavelength shifts based on first solar measurements for both OMPS NM (-0.14nm) and NP SDRs (-0.09nm).
- Solar and wavelength updates for three pixel offset error for OMPS NM SDR.
- Minor solar and wavelength updates for nadir macro-pixels, 4/7/2023.
- Minor sample table update for macro-pixel #177 is in Mx 8, July 13, 2023.
- Correction to OMPS NM SDR Solar Tables to 1 AU June 13, 2023.
- Better Jacobian for OMPS NM Straylight Corrections.
 - ADR 10360 has been opened for the OMPS NM SDR Straylight correction. A new table was implement on 6/26/2023. It improves performance but does not include the contributions from radiances longward of 380 nm.



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





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









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.



- The purpose of generating Soft-Calibration Adjustments for N21 V8TOz is to make its retrievals close to those from current operational NPP/N20 V8TOz.
- 13 consecutive days' (Jul. 01~Jul.13, 2023) 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.







Step2 Residuals by channel before Soft Calibration







Step2 Residuals by channel before Soft Calibration




















- 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	Туре	Description	
ErrorFlag		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
		High $SO_2 - 5$	SO_2 Index > 4 σ
		Non-Convergence – 6	Algorithm does not converge
		Large Residual – 7	Absolute residual > 32
EclipseFlag*		Bad Radiances – 8	Negative or missing radiances (Partial Granule Fix)
		0 – Good, 1 – Eclipse	Solar Eclipse Condition

NOAA-21 Calibration/Validation Maturity Review



Increased error flags for 4 and 5 are under investigation. There are two known contributions. One is particle events in the SAA and auroral ozone, combined with the smaller FOVs (less aggregation). The other is from the use of preliminary values to generate the SO2 Index error flag. The SDR Team is also looking at improvements to the stray light correction.







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







Dust and Smoke over Africa from OMPS NPP / N20 / N21 for July 5, 2023.



Percentage

Zonal Mean Reflectivity Differences to NOAA NPP-op



Difference



Difference



Comparisons of NPP Overpass to Dobson Stations, Mauna Loa HI



NOAA-21 Calibration/Validation Maturity Review



Comparisons of NPP Overpass to Dobson Stations, Boulder CO



NOAA-21 Calibration/Validation Maturity Review



Comparisons of NPP Overpass to Dobson Stations, Lauder NZ





 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.		Examine 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.



Documentations (Check List, 1 slide)

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)	



Beta Maturity End State	Assessment
Product is minimally validated, and may still contain significant identified and unidentified errors	NDE I&T product has significant errors from an error in creating the prelaunch Instrument Radiance Table.
Information/data from validation efforts can only be used to make initial qualitative or very limited quantitative assessments regarding product fitness- for-purpose	Ozone values should only be used for qualitative assessment due to instrument table error.
Documentation of product performance and identified product performance anomalies, including recommended remediation strategies, exists	New RT Instrument and Soft Calibration Adjustment Tables will be delivered to advance to Provisional Maturity. The new RT Instrument Table is in NDE I&T as of April 7, 2023.



Provisional Maturity End State	Assessment
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 select locations, periods, and associated ground truth or field campaign efforts.	Total Column Ozone product performance with the latest soft calibration adjustment table is good between 35S and 35N. Errors outside of the that region increase to 3%. The new soft calibration adjustment table will be delivered this month.
Product analyses are sufficient for qualitative, and limited quantitative, determination of product fitness-for-purpose.	Comparisons to NOAA-20 and S-NPP document the performance relative to expected behavior.
Documentation of product performance, testing involving product fixes, identified product performance anomalies, including recommended remediation strategies, exists.	The primary area for improvement is in the OMPS NM SDR Straylight OOR/B correction. The OMPS SDR Team is aware of the deficiency. The Ozone Team is investigating methods to improve performance for smaller FOVs.
Product is recommended for potential operational use (user decision) and in scientific publications after consulting product status documents.	Operational applications should only use products within 35° of latitude of the Equator. Other regions can be used in testing and offline studies for validation and comparisons.



Conclusions, Caveats and Path Forward at Provisional

- The NOAA-21 OMPS NM SDRs have improved performance as of the end of June 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 whether 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.



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