



Read-me for Data Users

MEMORANDUM FOR: The JPSS Program Record
SUBMITTED BY: JPSS OMPS Ozone Team Lead, Lawrence E. Flynn
CONCURRED BY: JPSS Algorithm Management Project Lead, Lihang Zhou
JPSS STAR Program Manager, Alisa Young
APPROVED BY: JPSS Program Scientist, Satya Kallura
SUBJECT: NOAA-20 OMPS Nadir Ozone Profile EDR Validated Maturity Status
REVIEW DATE: 5/27/2021
EFFECTIVE DATE: 6/30/2021 (Anticipated)

1. Background:

The Joint Polar Satellite System-1 (JPSS-1) was successfully launch on November 18, 2017 and renamed NOAA-20 after reaching polar orbit. With the same design as that of the Suomi NPP OMPS Nadir Sensors, the NOAA-20 OMPS consists of two spectrometers each with different spectral and spatial coverage. The OMPS Nadir Mapper (NM) SDR has spectral coverage from 300 nm to 380 nm with 196 channels and 1.1-nm bandpass. The OMPS Nadir Profiler (NP) SDR has spectral coverage from 250 nm to 310 nm with 150 channels and 1.1-nm bandpass. The OMPS nadir suite provides global measurements of total ozone, ozone profile, sulfur dioxide, UV reflectivity and an aerosol index.

Forty-eight days after launch, on January 5, 2018, the NOAA-20 Ozone Mapper Profiler Suite (OMPS) opened its door and started collecting science data. The initial data was in a high-spatial-resolution limited-spectra mode and was not compatible with the operational EDR algorithms. Since February 13, 2018 the instrument has been operated in a medium resolution mode and the NDE processing of the IDPS SDRs has created ozone EDR products.

The OMPS Ozone EDR team consists of experts from NOAA, NASA, IMSG, and industry partner Raytheon. The team has been working OMPS EDR pre- and post-launch calibration and validation for the Total Column Ozone EDRs from the V8TOz and V8TOS algorithms, and the Ozone Profile EDRs from the V8Pro algorithm as processed operationally at NDE.

The V8Pro algorithm uses eight channels from 253 nm to 306 nm from the OMPS NP and four channels from 313 nm to 372 nm from the OMPS NM to create estimates of the vertical ozone profile in 21 layers (~3-km each). The Ozone EDR Team recommends that the NOAA-20 OMPS V8Pro EDR advance to validated maturity.

2. Validated maturity stage definition:

- 1) Product performance has been demonstrated over a large and wide range of representative conditions (i.e., global, seasonal).
- 2) 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.
- 3) Product analyses are sufficient for full qualitative and quantitative determination of product fitness-for-purpose.
- 4) Product is ready for operational use based on documented validation findings and user feedback.

- 5) Product validation, quality assurance, and algorithm stewardship continue through the lifetime of the instrument.

3. **Justifications for declaring OMPS EDR data products validated maturity:**

The OMPS SDR and EDR team members have been analyzing the OMPS science RDR, telemetry RDR, SDR and GEO and EDR data products for the last nineteen months. Based on their analysis the following assessments of the OMPS NM and NP SDRs and the V8Pro EDR products were compiled:

- The SDR team reported that the performance for the SDRs met provisional maturity starting on July 2, 2018. The SDR noise level are as expected and weekly updates are used to maintain them adequately to meet EDR precision requirements. Biweekly updates to the wavelength scale are provided to track the annual cycle. Additional improvements on the path to validated maturity are described in the OMPS NP Validated Maturity Briefing and Readme. Please see the caveats in those documents and the memo of record from March 20, 2018 and further caveats on the SDRs in this memo;
- The NOAA STAR EDR team has successfully used the SDR data in V8Pro ozone profile retrievals and are generally positive about the measurement quality;
- The product performances are now close to requirements for most parameters globally.;
- The product error flags are functioning as designed and are identifying deficient products and compromised viewing conditions with frequencies as expected;
- The NOAA-20 V8Pro EDR products from NDE and STAR off-line processing using the new NOAA-20 OMPS NP SDR (Version 4) were compared to S-NPP EDR products – NOAA-20 ozone results are similar to those for S-NPP;
- On-orbit SDR radiometric biases were estimated based on comparisons with Suomi NPP OMPS, EOS Aura OMI and NOAA-19 SBUV/2 EDR measurement residuals and retrieval product sensitivities. These were used to generate the initial EDR soft calibration adjustments. Further rounds of adjustments will be constructed and provided as the SDRs are modified for the problems and updates as noted herein;
- The EDR Team has delivered revised algorithms and tables to NDE for implementation in the operational processing system to improve the product quality. The v3r3 for V8Pro is operationally at NDE. The latest code changes and a new soft calibration adjustment table, v4r0, have been delivered to NDE and are in testing on the I&T string. The code contains several areas of improvement. Details are provided in Appendix C. A one-line code correction as provided a direct patch to NDE and they were able to implement it in the v4r0 in the I&T string. The Validated Maturity products will commence production and regular distribution once two conditions are met: (a) the V8Pro v4r0 delivery with the wavelength-scale code patch and new adjustment table is implemented at NDE, and (b) the NOAA-20 OMPS NP SDR correction is implemented at IDPS for the Solar In-Band Stray Light (IBSL).
- NOAA-20 OMPS Nadir Ozone Profile EDR data products for the full Earth after these updates can be used for applications and science. The NOAA-20 results for V8Pro v4r0 ozone profiles are within $\pm 5\%$ of those from S-NPP V8Pro v4r0 for global zonal means.

The presentations and Readmes for the OMPS SDR and V8Pro Ozone EDR products justifying their advances to validated maturity can be found at

<https://www.star.nesdis.noaa.gov/jpss/AlgorithmMaturity.php>

4. NOAA-20 OMPS Ozone EDR Validated maturity caveats

The following caveats are provided to EDR product users:

- A fix to the calibration constant computations for the OMPS NP SDR cross-track macropixels (DR 8615) was implemented at IDPS on July 2, 2018;
- The OMPS NM SDR program dropped scans when the RDRs contain 16 scans in a granule. A fix to correct this problem (CCR 18-3829) transferred to operations with Block 2.1 Mx3 on September 24, 2018;
- The smaller FOVs for the NOAA-20 V8Pro EDRs lead to poorer performance (noisier retrievals from transient spikes) in the South Atlantic Anomaly (SAA) than is seen for the S-NPP V8Pro EDRs. The SAA flag is not set for some of the affected retrievals beyond the edges of the currently defined region. The V8Pro v3r3 implements an information concentration and outlier screening process to reduce the measurement noise in the selected channels and identify the presence of outliers;
- While working on the next step to reduce the effects of noise and outliers, a discretization error from the nonlinearity correction formulation was discovered. The error creates solar zenith angle dependent biases in the measurements for the two shortest profile channels which provide information at the top of the retrieval. This discretization error was reduced to a negligible level by implementing a new flight nonlinearity table and a new ground radiance calibration table (ADR 8730). The new table was provided along with new calibration coefficients. This update was implemented in IDPS on December 4, 2018;
- The first round of updates to the NOAA-20 OMPS sample tables do not provide good enough matchups between the NP and NM FOVs as needed by the V8Pro algorithm. A full set of SDR tables (including wavelength, solar, and stray light) have been developed for use with a new OMPS NM flight sample table. These new SDR and sample tables have been in use since April 19, 2019;
- The V8Pro EDR products described in the Provisional Maturity Review and Appendix B (v3r3) began use in NDE on January 22nd 2020. The NOAA-20 V8Pro adjustments give good agreement with the S-NPP V8Pro within 20° of latitude of the Equator but the retrievals deviate outside that range;
- The OMPS NP SDR tables have been tuned for on-orbit performance. DR9093/CCR 19-4638 provides LUT updates for NOAA-20 OMPS NM & NP SDRs to reach Validated Maturity. This delivery has been completed.
- The S-NPP OMPS NP SDRs were affected by small but significant degradation in the optical throughput and by an annual cycle in the wavelength scale exceeding the stability requirements. The wavelength scale variations for S-NPP led to the use of biweekly updates to the solar and wavelength scale tables. The SDR team has implemented biweekly updates for the OMPS NP wavelength scale and solar to account for the annual cycle in wavelength scale. The SDR and EDR teams monitor the NOAA-20 OMPS NP SDR performance to see if degradation changes are present at levels requiring calibration updates. The SDR Team is also investigating how to best include solar activity in the bi-weekly calibration updates.
- There was an open question on the accuracy of the NOAA-20 OMPS NP SDR wavelength scale. New wavelength scale and calibration coefficient tables were implemented in IDPS starting on August 21, 2020.
- The V8Pro EDR products described in the Validated Maturity Review and Appendix C (v4r0) is at NDE I&T as of the writing of this memo. This new version includes a correction for the NOAA-20 OMPS NP wavelength scale calculation and soft calibration adjustments to force NOAA-20 V8Pro to agree with S-NPP V8Pro.

- The current (5/2021) NOAA-20 OMPS NP SDRs do not yet apply the solar IBSL corrections, so the performance for retrievals in the Northern Hemisphere for SZAs greater than 62° will deviate from the truth and differ by over -10% from the S-NPP results for the upper half of the retrievals. This correction is ready for transition to IDPS operations with the next build.

5. Path Forward

The team will work to continue with the following planned calibration and validation tasks to further improve the OMPS EDR data products:

- 1) Provide new bandpass tables with adjustments for the actual channel locations relative to each instrument's wavelength scale to better account for interpolation effects.
- 2) Provide new calibration adjustment tables to account for the NPP Wavelength Scale shift present in the operational S-NPP OMPS NP SDRs for 3/2021 which were used to generate the NOAA-20 soft calibration results currently provided to NDE.
- 3) Investigate polarization sensitivity differences as a possible source of latitude-dependent biases for between S-NPP and NOAA-20 for the longer V8Pro wavelength channels.
- 4) Regularly update the V8Pro soft-calibration adjustments to account for degradation of the throughput for the OMPS NP instruments.
- 5) Continue to compare non-Equatorial regional means, zonal means and global statistics for V8Pro EDRs with those for S-NPP. Compare ozone profile products to ground-based measurements by using overpass data sets for Umkehr and Ozonesonde stations. Compare BUFR products to current assimilation forecasts;
- 6) Track the impact of continued improvements in the S-NPP and NOAA-20 SDRs as planned by the SDR and EDR teams with particular attention to wavelength scales or bandpass changes and channel locations and interpolation which might affect the observed latitude dependence; and
- 7) Provide deliveries of adjustment tables and code changes for V8Pro to NDE as SDR knowledge improves, validation results are analyzed and throughput degradation is quantified.

Additional information is available in the OMPS V8TOz and V8Pro algorithm theoretical basis documents (ATBDs) and the SDR beta maturity review briefing, which can be accessed at:

<https://www.star.nesdis.noaa.gov/jpss/Docs.php>

and

<https://www.star.nesdis.noaa.gov/jpss/AlgorithmMaturity.php>

NOAA-20 OMPS SDR near-real-time status and performance monitoring web page are available by using the following password protected websites:

https://www.star.nesdis.noaa.gov/icvs-beta/status_J01_OMPS_NP.php

https://www.star.nesdis.noaa.gov/icvs-beta/status_J01_OMPS_NM.php

NOAA-20 OMPS SDR near-real-time status and performance monitoring web page are available at the open website:

<https://www.star.nesdis.noaa.gov/icvs/index.php>

NOAA-20 OMPS EDR near-real-time status and performance monitoring web pages are available at the following websites:

Archive https://www.class.ncdc.noaa.gov/saa/products/search?datatype_family=JPSS_OZONE

Operations <http://www.ospo.noaa.gov/http://www.ospo.noaa.gov/Products/atmosphere/index.html>

Long-term <https://www.star.nesdis.noaa.gov/smcd/spb/OMPSDemo/proOMPSbeta.php>

Daily maps https://www.star.nesdis.noaa.gov/jpss/EDRs/products_ozone.php

Activity <https://ozoneaq.gsfc.nasa.gov/omps/n20/activity>



Read-me for Data Users

Points of Contact:

Name: Lawrence E. Flynn, EDR Team Lead

Email: Lawrence.E.Flynn@noaa.gov

Phone: 301-683-3612

Vaishali Kapoor, Ozone Product Area Lead

Vaishali.Kapoor@noaa.gov

301-683-3246

Timeline of V8Pro Versions for NOAA-20 OMPS processing:

N20 V3R2 started on August 16th, 2018.

N20 V3R3 started from NDE OPS starting on January 22nd, 2020 with the following granule:

V8PRO-EDR_v3r3_j01_s202001221544286_e202001221545060_c202001221857090.nc

N20 V4R0 is on the NDE Development as of 5/1/2021.

Appendix A. Updates to Key items from OMPS SDR Provisional Memo.

- 1) There is a sub-optimal match in the CCD pixels for the OMPS-TC and OMPS-NP sample tables. The OMPS-TC and OMPS-NP are not viewing exactly the same spatial region within each FOV. A better alignment could be achieved. For example if a bright cloud fills one OMPS-TC FOV pixel but is cloud-free in an adjacent FOV pixel the OMPS-NP alignment will sample both the cloud and cloud free pixel. The alignment difference is small but could be significant in some cases. The difference in field of view will sometimes in the worst case combine the bright scene and dark scene in the NP pixel. There is a report on this issue, DR_8617, “FOV Mismatch between N20-OMPS-TC and N20-OMPS-NP”. This was corrected as of April 19, 2019.
- 2) In July 2018, the science team discovered the OMPS-NP non-linearity correction is causing a discretization error for low signal levels. The error is causing a signal level dependent 2% error at shorter channels. Our analysis shows the error can be removed by uploading a new non-linearity table to the NOAA-20 and updating the calibration coefficient file in the IDPS. DR_8730 was opened on this topic. This was corrected as of February 2019.
- 3) Check for degradation in the OMPS-NP shortest spectral region. Monitoring is on-going. Solar reference measurements are made every six months.

Appendix B. V8Pro Upgrades in v3r3

A. Dual Adjustment Tables

- Provides Old (Current) and New (Updated) soft calibration tables with the option to interpolate between them to smooth the transition at the request of data assimilation applications. File names will have creation dates.

B. Metadata improvements.

- Additional fields are added to metadata to be consistent with NDE requirements and to provide better information. These include the NDE production site, NDE production environment, and the adjustment table’s file name.

C. Area-Weighted FOV Averages and Allow High Resolution OMPS NM SDRs

- When the NOAA-20 OMPS NM SDR goes to [10,10,10,10, 5,10, 5,10,10,10,10] or to [5, 5, 5, 5, 5, 5, 5, 5, 5,10, 5, 5, 5, 5, 5, 5, 5, 5, 5] pixel aggregation, we will want to have

area-weighted values computed in the glueware. This refinement provides the code to calculate and use the relative sizes of the FOVs.

D. Remove the use of 340 nm channel for reflectivity.

- Code updates were made to switch from 340 nm channel to 331 nm channel for some reflectivity calculations for consistency with the NASA V8Pro implementation.

E. Code Fixes

- Averaging Kernels: Changes OMPS V8Pro product configuration for the averaging kernels to agree with the SBUV/2 relative response ones.
- Mixing Ratios: Corrects inconsistency in height order of mixing ratio amount and pressure.
- Surface Pressure: Extends Terrain Pressure maximum and minimum to include the Dead Sea and Mt. Everest.
- Descending Orbits: Descending orbit data were not processed – fixed by changing the geolocation corner order in the Glueware.

F. Change to handle OMPS NM SDR sizes up to 30 scans x 140 cross-track FOVs per granule.

- This refinement will read in the SDR granule sizes and properly select OMPS NM SDR FOVs for 5, 15 or 30 scan granules with up to 140 cross track granules to match up with the OMPS NP EDR FOV.

G. Outlier Detection Filter and Information Concentration (F&IC)

- Implements a combination of median filter and 10- to 12-wavelength polynomial fits of the radiance / irradiance ratios for the shorter ozone profile channels to reduce measurement noise, remove outliers and identify PMCs. A flag is set if the radiances have too many outliers.

Table 1: V8Pro Profile Error Code and Descriptions

Profile Error Code	Description
0.0	Good retrieval
1.0	SZA > 84 degrees
2.0	Step3O3 – Profile Total > 25 DU
3.0	Average Final Residual for retrieval channels > threshold
4.0	Final residue greater than 3 times instrument error
5.0	Retrieved - a priori greater than 3 times a priori error
6.0	Non-convergent solution
7.0	Stray light anomaly
8.0	Initial residue greater than 18.0 N-value units or upper level profile anomaly
9.0	Total ozone algorithm failure
20.0	Thresholds on number of deviations from polynomial fit.
40.0	+20 for >30%, +40 for >60%.

Appendix C. V8Pro Upgrades in v4r0

A. Modifications for J02

- Modified scripts and codes to run J02 input with smaller OMPS NM FOVs.
- Added placeholders with baselined values for required J02 tables and ancillary files.

B. Improved Fidelity for Slit Function Models

- Used new instrument-dependent wavelength bandpass responses to generate radiative transfer tables.
- Increased the fidelity of the internal bandpass model. It is now using the SDR-team provided instrument bandpass weights in the single scattering calculations.
- New tables are under development to improve the modeling of the as-interpolated channel measurements. This will become v4r1.

C. Revised Soft Calibration Adjustments

- Changed S-NPP adjustments to generate zero bias aerosol for the Equatorial Pacific. Made adjustments for instrument throughput degradation as used in the Climate Data Records.
- Set NOAA-20 adjustments to match S-NPP for 3/2021 for all channels. Set J02 adjustments to zero for initial beta processing.

D. Naming Convention

- Renamed tables for consistency with npp/j01/j02 NDE naming convention.

E. Wavelength Scale Error

- A one-line code error in the NOAA-20 wavelength scale calculation was corrected. This error produced bad wavelength scales for the NOAA-20 OMPS NP processing. This correction was delivered as a patch directly to NDE for the v4r0 in April 2021.

F. New Soft Calibration Adjustment Table

- After applying the one-line code fix, a new soft calibration adjustment table was created using the March 2021 data comparisons between S-NPP and NOAA-20 V8Pro for the Equatorial zone. This table was included in the April patch.

Appendix D. Solar In-Band Stray Light (IBSL) Model

Developed by L.-K. Huang, NASA GSFC (SSAI).

NOAA-20 OMPS Nadir Profiler In-Band Stray Light Characterized with comparison of a priori profile residues between SNPP and N20IBSL is given in terms of albedo values:

$$IBSL = AvgPrfile(scsea) / \{AvgScaleFactor(lamda) * [1 + DriftRate(lamda) * (YearFrac - y18m2)] * [C0 + C1 * (scsaa - scsaa21)]\}$$

where scsea is the Spacecraft Centered Solar Elevation Angle in degrees near the North Pole, scsaa is the spacecraft Centered Solar Azimuth Angle at SCSEA=-2.5 degrees near the North terminator.

Wavelength (nm)	252.040	273.700	283.160	287.730	292.360	297.640	
AvgScaleFactor	1.08680	0.794994	1.09403	0.996082	0.986087	0.923263	
DriftRate (per year)	-0.08887	0.08599	0.02556	0.04522	0.01692	0.02873	
y18m2	2018.1383						
SCSAA Dependence coefficients C0 and C1, scsaa21	1.01454	0.0156717	21.0				
SCSEA AvgPrfile							
-32.5	-3.57e-10	-32.0	-2.46e-09	-31.5	3.71e-08	-31.0	1.25e-07
-30.5	2.57e-07	-30.0	4.17e-07	-29.5	5.83e-07	-29.0	7.57e-07
-28.5	9.77e-07	-28.0	1.27e-06	-27.5	1.70e-06	-27.0	2.29e-06
-26.5	2.93e-06	-26.0	3.55e-06	-25.5	4.07e-06	-25.0	4.39e-06
-24.5	4.58e-06	-24.0	4.69e-06	-23.5	4.73e-06	-23.0	4.73e-06
-22.5	4.70e-06	-22.0	4.66e-06	-21.5	4.61e-06	-21.0	4.55e-06
-20.5	4.49e-06	-20.0	4.43e-06	-19.5	4.38e-06	-19.0	4.32e-06
-18.5	4.28e-06	-18.0	4.23e-06	-17.5	4.20e-06	-17.0	4.15e-06
-16.5	4.11e-06	-16.0	4.06e-06	-15.5	4.02e-06	-15.0	3.98e-06
-14.5	3.93e-06	-14.0	3.89e-06	-13.5	3.86e-06	-13.0	3.83e-06
-12.5	3.81e-06	-12.0	3.80e-06	-11.5	3.79e-06	-11.0	3.78e-06
-10.5	3.75e-06	-10.0	3.73e-06	-9.50	3.71e-06	-9.00	3.69e-06
-8.50	3.66e-06	-8.00	3.64e-06	-7.50	3.62e-06	-7.00	3.60e-06
-6.50	3.58e-06	-6.00	3.56e-06	-5.50	3.55e-06	-5.00	3.53e-06
-4.50	3.51e-06	-4.00	3.49e-06	-3.50	3.47e-06	-3.00	3.44e-06
-2.50	3.36e-06						



Appendix E. Key items from OMPS SDR Validated Memo.

- **Timeline of SDR Improvements**
 - See SDR Readme's.
- **Three RFAs After Validated Maturity**
 - **Links to bandpass and wavelength scale datasets** → provided by SDR team 6/2020.
 - **CCR on OMPS NP Wavelength Scale, Solar and calibration coefficients** → Transfer to IDPS Operations 8/21/2020.
 - **IBSL Investigation and Correction Plan** → The solar intrusion correction will be implemented at IDPS operations with the next build.

https://drive.google.com/drive/folders/13F5S517ntc_aouZodQgYr8djkuHSPOc