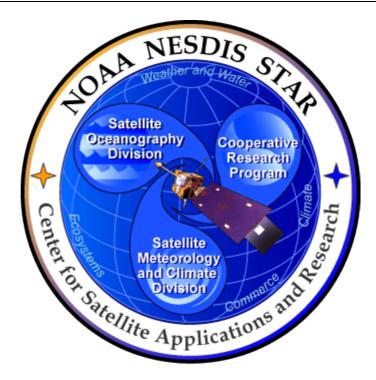
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NOAA NESDIS CENTER for SATELLITE APPLICATIONS and RESEARCH

The NOAA Suomi-NPP Data Exploitation (NDE) Version 8 Ozone Profile (V8Pro) Environmental Data Record (EDR) NDEV8P

External Users' Manual

Version 1.1



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TITLE: NDE VERSION 8 OZONE PROFILE EDR EXTERNAL USERS' MANUAL VERSION 1.0

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DOCUMENT HISTORY DOCUMENT REVISION LOG

The Document Revision Log identifies the series of revisions to this document since the baseline release. Please refer to the above page for version number information.

	DOCUMENT TITLE: External Users Manual Template					
	DOCUMENT CHANGE HISTORY					
Revision No.	Date	Revision Originator Project Group	CCR Approval # and Date			
1.0	March 10, 2016	STAR JPSS Ozone Product				

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LIST OF CHANGES

Significant alterations made to this document are annotated in the List of Changes table.

DOCUMENT TITLE: External Users Manual Template

LIST OF CHANGE-AFFECTED PAGES/SECTIONS/APPENDICES

				-	
Version Number	Date	Chang ed By	Page	Section	Description of Change(s)
1.0	09/10/16	Flynn	All	All	Created Version 1.0

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PRODUCTS

This is an External Users Manual (EUM) document describing the operational NOAA NDE Ozone Profile Environmental Data Record product and output file. The NDEV8P provides the Ozone Mapping and Profiler (OMPS) Ozone Profile bundled product as created by the Version 8 Ozone Profile retrieval algorithm developed at NASA GSFC.

The work to transition the algorithm to NOAA operations was completed as part of the NOAA JPSS Product Development, Calibration and Validation program led by the NOAA NESDIS Center for Satellite Applications and Research (STAR). It will be delivered to the Suomi NPP Data Exploitation (NDE) team and integrated into the NDE Data Handling System (DHS) where it will be run in a pre-operational manner. After a preliminary testing period, the NDE DHS will, in turn, be delivered to the Office of Satellite and Product Operations (OSPO) to be run operationally.

The intended users of this EUM are end users of the operational output products and files, and the product verification and validation (V&V) teams. The purpose of the EUM is to provide product users and product testers with information that will enable them to acquire the product, understand its features, and use the data. External users are defined as those users who do not have direct access to the processing system (those outside of the OSPO and NDE). The output files are defined as those leaving the NDE DHS (running within ESPC) as opposed to those that are output by the V8PRO processing, but available only internally within the NDE.

Product Overview

Product Requirements

All NDEV8P basic and derived requirements are available in the V8PRO Requirements Allocation Document (RAD). These requirements identify the users and their needs with respect to file content, format, latency, and quality. They are based on the Level 1 Requirements for Ozone Profile EDRs from the JPSS program.

Product Team

The NDEV8P Development product team consists of members from STAR, NASA GSFC, and OSPO. The roles and contact information for the different product team members are identified in Table 1-1.

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Team Member	Organization	Role	Contact Information
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Robert Lindsay	OSPO	Programmer -	Email: robert.lindsay@noaa.gov
		NDE	

Table 1-1 Product Team Members

Product Description

The NDEV8P product was developed to generate Ozone Profile estimates from a discrete set of 13 measurements of backscattered ultraviolet radiances in the 250 nm to 380 nm range. It creates a 21-layer ozone retrieval along with measurement residuals, error flags and other retrieval parameters. In addition to the ozone profile retrieval, it also makes total ozone estimates, and produces effective UV reflectivity, absorbing aerosol index values and retrieval information such as measurement sensitivities and residuals and retrieval efficiency factors. The algorithm processes all daytime OMPS Nadir Profiler Sensor Data Records (SDRs). Details on the content of the NDEV8P external output files are provided in section 1.3.

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Product History

The NDEV8P is a new implementation of the Version 8 Ozone Profile retrieval algorithm developed by NASA GSFC for the Solar Backscatter Ultraviolet (SBUV(/2)) series of instruments and refined for use with the NASA EOS Aura Ozone Monitoring Instrument (OMI). NOAA has previously implemented this algorithm operationally to create products from measurements made by the NOAA POES SBUV/2 instruments.

This product replaces the current operational IDPS Ozone Profile IP and planned EDR products (IMOPO, OONPO and INPAK). The IDPS and NDE products meet the JPSS Level 1 requirements. The NDE product will also be consistent with the existing NOAA SBUV/2 records.

Product Access

All NDEV8P output data files will be made available by the NDE DHS on the NDE data distribution server at ESPC in a near real time manner. For access to this server, information about data files, and associated documentation, the NDEV8P Product Area Lead (Ozone PAL) should be contacted (see Table 1-1).

The NESDIS Policy on Access and Distribution of Environmental Data and Products is provided at: http://www.ospo.noaa.gov/Organization/About/access.html. Users need to fill out the Data Access Request Form located on this site and submit to the PAL with a copy to nesdis.data.access@noaa.gov. This address provides the OSPO Data Access Team a copy of the correspondence. Once the request is approved by the OSPO management the data will be delivered by the Data Distribution System (DDSProd) currently distributing the ESPC data products and later by the Product Distribution and Access (PDA) system. The ESPC Data Distribution Manager, Donna McNamara (donna.mcnamara@noaa.gov) should be contacted for any data accessibility and data distribution problems. The data format is defined in the Table 1.2

In order to obtain the near real time data users need to fill out the Data Access Request Form located on <u>http://www.ospo.noaa.gov/Organization/About/access.html</u> and submit to the PAL with a copy to <u>nesdis.data.access@noaa.gov</u>. CLASS will be archiving the V8PRO data products for distributing to the non-real-time users. NDE pushes the data to CLASS with the associated metadata in the standard formats. CLASS will archive the V8PRO product in netCDF4 format with associated metadata.

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Table 1-2 describes the external distributed NDEV8P file and Table 1-3 lists its content. Details of the derivation of all of the products are described in the NDE Version 8 Ozone Profile Algorithm Theoretical Basis Document. Table 1-4 decodes the error flag values.

Table 1-2 NDE Ozone Profile File

File	Description	Format	Size/file
V8PRO-	This is the granule output	netCDF4	0.2 MB/granule file,
EDR_v1r0_npp_s20160	file containing all the		~1100 files/day
1120127494_e2016011	derived variables of the		
20128268_c201603221	NDEV8P product.		
503000.nc	-		

Table 1-3 Ozone Profile Output Granule File Content

Name	Туре	Description	Dimension	Units	Range
Latitude	32 bit Float	Latitude	5 x 5	Degrees	-90 ~ 90
Longitude	32 bit Float	Longitude	5 x 5	Degrees	-180 ~ 180
LatCorner	32 bit Float	Latitude	4 x 5 x 5	Degrees	-90 ~ 90
LonCorner	32 bit Float	Longitude	4 x 5 x 5	Degrees	-180 ~ 180
RelativeAzimuthAngl e	32 bit Float	The Relative Azimuth angle	5 x 5	Degrees	-180 ~ 180
SolarAzimuthAngle	32 bit Float	Solar Zenith Angle	5 x 5	Degrees	0 ~ 180
SolarZenithAngle	32 bit Float	Solar Zenith Angle	5 x 5	Degrees	0 ~ 180
ViewingAzimuthAngle	32 bit Float	The satellite azimuth angle	5 x 5	Degrees	0 ~ 180
ViewingZenithAngle	32 bit Float	The viewing zenith angle	5 x 5	Degrees	0 ~ 180
UVAerosolIndex	32 bit Float	Aerosol Index	5 x 5	Unitless	-100~ 100
AlgorithmFlag_TO3	32 bit Intege r	Algorithm Flag	5 x 5	Unitless	0 ~ 10
Ascending_Descendi ng	32 bit Intege r	1=Descending, 0=Ascending	5 x 5	Unitless	0~ 1

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AverageSolutionResi dual	32 bit Float	Average of residuals	5 x 5	Nvalue	0~ 20
AveragingKernel	32 bit Float	Averaging kernel matrix at 20 layers	20 x 20 x 5 x 5	DU/DU	-500~ 500
ChannelBandpassFW HM	32 bit Float	The FWHM band width assumption	13	Nanomet ers	0.2~ 50
CloudPressure	32 bit Float	Cloud Pressure	5 x 5	hPa	10~ 1500
ColumnAmountO3_P rofile	32 bit Float	Ozone Profile Column Sum	5 x 5	Dobson Units	0~ 10000
ColumnAmountO3_T O3	32 bit Float	Step 3 ozone	5 x 5	Dobson Units	10~ 1000
CorrelationLength	32 bit Float	The correlation length	1	Unitless	0~ 81
EffectiveCloudFractio n	32 bit Float	Radiative Cloudfraction	5 x 5	Unitless	0~ 100
ErrorApriori	32 bit Float	The apriori error covariance matrix assumption	1	Unitless	0~ 10
ErrorCode_Profile	32 bit Intege r	Profile Return Code	5 x 5	Unitless	0 ~ 19
ErrorCode_TO3	32 bit Intege r	Error flag from the Total ozone computation	5 x 5	Unitless	0 ~ 10
ErrorMeasurement	32 bit Float	The measurement error	10	Unitless	0~ 10
FINALRESIDUAL	32 bit Float	Final Residuals from solution profile	10 x 5 x 5	Unitless	-100~ 100
INITIALRESIDUAL	32 bit Float	Initial Residuals from solution profileprofile	10 x 5 x 5	Unitless	-100~ 100
IndexLongestChannel	32 bit Intege r	Index of longest channel used	5 x 5	Unitless	1 ~ 500

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		in retrieval			
InformationContent	32 bit Float	Information Content, the trace of the averaging kernel	5 x 5	Unitless	0~ 20
JACOBIAN	32 bit Float	Jacobian from internal forward model	20 x 20 x 5 x 5	Delta_nva lue / Delta_lay er_ozone	-1000~ 1000
MidTime	64 bit Float	Elapsed time in seconds since Jan 1, 1958 including leap seconds	15	Microsec onds	1.0~ 1.0E12
NValue	32 bit Float	Measure Nvalues at all channels	13 x 5 x 5	Nvalue	10~ 5000
NumberIterations	32 bit Intege r	Number of iterations for Convergence	5 x 5	Unitless	1 ~ 100
NvalueAdjustment	32 bit Float	Computed Nvalue soft calibration adjustment	13 x 5	Nvalue	-3~ 3
O3Apriori	32 bit Float	Apriori Ozone Profile	21 x 5 x 5	Dobson Units	0~ 1000
O3BelowCloud	32 bit Float	Ozone below cloud estimate	5 x 5	Dobson Units	0~ 100
O3FINAL	32 bit Float	Ozone Solution Profile	21 x 5 x 5	Dobson Units	0~ 1000
O3Initial	32 bit Float	First Guess Ozone Profile	21 x 5 x 5	Dobson Units	0~ 1000
O3MixingRatio	32 bit Float	ozone volume mixing ratio	15 x 5 x 5	PPMV	0~ 1000
Pressure	32 bit Float	The pressure at the bottom of each layer in the solutionprofile	21	hPa	0.1~ 1013.25
PressureMixingRatio	32 bit Float	The pressure levels of the volume mixing	15	hPa	0.5~ 50.0

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		ratio profile			
Reflectivity331	32 bit Float	Computed reflectivity at the 331nm channel	5 x 5	Unitless	0~ 100
Reflectivity340	32 bit Float	Computed reflectivity at the 340nm channel	5 x 5	Unitless	0~ 100
Reflectivity380	32 bit Float	Computed reflectivity at the 380nm channel	5 x 5	Unitless	0~ 100
Residual_TO3	32 bit Float	Residuals from total oz calculation	5 x 5 x 5	Dobson Units	-100~ 100
SnowIceFlag	32 bit Intege r	Snow Ice flag from Climatology	5 x 5	Unitless	1 ~ 100
StepOneO3	32 bit Float	Step 1 ozone	5 x 5	Dobson Units	10~ 1000
StepTwoO3	32 bit Float	Step 2 ozone	5 x 5	Dobson Units	10~ 1000
SurfaceCategory	32 bit Intege r	Scene Type from Lookup Table	5 x 5	Unitless	1 ~ 100
TemperatureClimatol ogy	32 bit Float	Temperature profile used in solution	21 x 5 x 5	Degrees Kelvin	100~ 400
TerrainPressure	32 bit Float	Terrain Pressure from lookup tables	5 x 5	hPa	100~ 1500
WaveLength	32 bit Float	The band centers for all channels	13	Nanomet ers	260~ 550
Wavelength_Profile	32 bit Float	The band centers for channels used in the profile oz computation	10	Nanomet ers	260~ 550
Wavelength_TO3	32 bit Float	The band centers for	5	Nanomet ers	260~ 550

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		channels used in the total oz computation			
dndo_TO3	32 bit Float	Ozone sensitivities	5 x 5 x 5	NValue/D obson Unit	-20~ 50
dndr_TO3	32 bit Float	Reflectivity sensitivities	5 x 5 x 5	NValue	0~ 600
quality_information	32 bit Intege r	granule quality information attributes	1	percentile	0~ 100
yearday	64 bit Float	The day of year	5 x 5	day	1~ 366

Table 1-4a Details of the V8Pro Total Ozone Error Code and Descriptions

Total Ozone Error Code	Description
0.0	Good retrieval
1.0	Bad Aerosol information
2.0	SZA > 84 degrees
3.0	380 nm residue greater than limit (Not Used)
4.0	Ozone inconsistency
5.0	SO2 Contamination
6.0	Step 1 ozone iteration did not converge
7.0	Any channel residue greater than 16 or bad radiance
8.0	Spare
9.0	Spare
+10.0	10 is added to the flag values to designate descending portions of the orbit. The unit's value is unchanged.

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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
+10.0	10 is added - to the flag values to designate descending portions of the orbit. The unit's value is unchanged.

Table 1-4b V8Pro Profile Error Code and Descriptions

ALGORITHM

Algorithm Overview

Radiation at the near–UV wavelengths is absorbed by ozone, such that the difference between the incoming and outgoing radiation can be related to the amount of ozone in the atmosphere. Radiation amounts at the eight shortest wavelength channels used in the V8PRO are absorbed by atmospheric ozone before reaching the surface, implying that radiation scattered back to the instrument came from a particular altitude range. Radiation at successively longer wavelengths penetrates deeper into the atmosphere before being completely absorbed by ozone, allowing for a measure of the ozone profile. In the Version 8 algorithm, the total ozone is also calculated as the sum of the retrieved profile ozone, rather than just from measurements at the four longest wavelengths, which do penetrate to the surface. This makes the total ozone less sensitive to the variations in surface reflectivity and scattering processes in the troposphere. TITLE: The NDE Version 8 Ozone Profile EDR External Users' Manual

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The NDEV8P product is generated from the Version 8 Ozone Profile algorithm (V8PRO). The V8PRO uses a new set of profiles for the *a priori* information leading to better estimates in the troposphere (where BUV measurements lack retrieval information) and to simplified comparisons of SBUV/2 and OMPS results to other measurement systems (in particular, the Umkehr ground-based O₃ profile retrievals which now use the same set of *a prioris*). The V8PRO has improved total O₃ retrievals from improved multiple scattering and cloud and reflectivity modeling. Some errors present in the V6A version will be reduced. These include a correction for 2% errors from previously ignoring the gravity gradient with height and elimination of 0.5% errors from low fidelity bandpass modeling. The V8PRO is also designed to allow the use of more accurate external and climatological data, to adjust for changes in wavelength selection, and to incorporate several *ad hoc* Version 6 algorithm improvements directly. Some components of the initial V8PRO implementation were optimized for trend detection. These are modified for use in operations but the algorithm has the flexibility to make these changes.

Input Satellite Data

Satellite Instruments

NDEV8P is a system operated within the NDE DHS by OSPO. It uses measurements from the Ozone Mapping and Profiler Suite (OMPS) Nadir Profiler (NP) and Nadir Mapper (NM) on the Suomi National Polar-orbiting Partnership (S-NPP) platform and will continue with OMPS on future satellites of the Joint Polar Satellite System (JPSS). S-NPP was launched on October 28, 2011. It is in a sun synchronous orbit with a 1:30 PM ascending-node orbit at an altitude of 829 km.

The OMPS NM instrument is a pushbroom spectrometer with a 2-dimensional CCD array detector. The telescope images a 105° cross-track FOV onto the array, providing full daily coverage of the sunlit Earth. It has 196 spectral bands covering the spectrum between 300 nm to 380 nm with 1.1 nm FWHM and 0.42-nm sampling. The instrument is highly flexible and is currently operated to aggregate approximately 20 spatial pixels into 35 cross-track bin and to integrate for approximately 7.8 S. This produces 50x50 km² size products at nadir. Plans for J-01 are to reduce both dimensions by a factor of three and create 103 cross track bins every 2.6 S with 17X17 km² size products at nadir.

The grating spectrometer and focal plane for total column measurements provide 0.42 nm spectral sampling across the wavelength range of 300 to 380 nm. The radiance/irradiance ratios for the four longer wavelengths used in the V8Pro EDR algorithm are obtained by interpolating the values at adjacent measurement wavelengths to provide them at the following wavelengths:

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[313, 318, 331.3, ,360.2, 380] nm ??

The OMPS NP instrument is a nadir-viewing double monochromator with 2-dimenstional CCD array detector. The same telescope provides the signal but only the central nadir 14° FOV is imaged on the detector. A dichroic element with a transition interval from 300 nm to 310 nm is used to split the signal into the NM and NP components. The NP has 147 bands with 0.42 nm spacing and 1.1 nm FWHM bandpasses from 250 nm to 310 nm. The radiance/irradiance ratios for the eight shorter wavelengths used in the V8Pro EDR algorithm are obtained by interpolating the values at adjacent measurement wavelengths to provide them at the following wavelengths:

[253, 273, 283, 288, 292, 298, 302, 306] nm ??

Satellite Data Preprocessing Overview

The OMPS Raw Data Records (RDRs) are processed at IDPS into Sensor Data Records (SDRs) by the OMPS NP SDR and OMPS NP geolocation and OMPS NM SDR and OMPS NM geolocation algorithms. This processing includes the geolocation and radiometric calibration of the raw sensor output. Details of the OMPS SDR algorithm are described in the JPSS OMPS SDR ATBD.

Input satellite data description

The NDEV8P algorithm uses the radiance and irradiance measurements provided in the OMPS NP and NM SDR and the geolocation and viewing geometry information provided in the OMPS NP and NM GEO. Table 2-1 provides a summary of the OMPS SDR and GEO parameters used by the algorithm.

Input	Туре	Description	Units/Valid Range		
Pixel-Leve	Pixel-Level Data Items				
satza	real	Satellite zenith angle	Degrees		
sza	real	Solar zenith angle	Degrees		
xphi	real	Relative azimuth angle between	Degrees		
		sensor and solar azimuth angles			
month	integer	Month of measurement	Month / 1 – 12		
day	integer	Day of month of measurement	Day		
seconds	long	Seconds in day of mesurment	Seconds		
	interger				
xlat	real	Latitude of measurement	Degrees / -90 – 90		

Table 2-1 OMPS SDR and GEO data used by the NDEV8P algorithm

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Input	Туре	Description	Units/Valid Range
xlong	real	Longitude of measurement	Degrees / -180 – 180
xm	real	Radiances for 26 sensor wavelengths	W/m ² -nm / 0 – 3x10 ⁷
Sflux	real	Solar flux for 26 sensor wavelengths	W/m ² -nm / 0 – 3x10 ⁷

Input Ancillary Data – Climatolgy and RT LUTs

The NDEV8P uses climatological values for Cloud Top Pressure, Snow/Ice Fields, Surface Pressure and for Ozone and Temperature Profiles. It also uses radiative transfer Look-Up Tables to provide estimates of the top-of-atmosphere radiance/irradiance ratios (and their sensitivities to ozone layer perturbations) for standard ozone profiles and a select array of viewing conditions. Table 2-2 provides a summary of the climatological and table parameters used by the algorithm.

Table 2-2 Satellite, Climatological and Table data used by the NDEV8P algorithm

File Type	No.	Filename	Content	Data Format
Control File	1	namelist.nml	Runtime parameters (generated by driver script)	ASCII
IDPS Granule File	2	SOMPS_npp_IDP STime [§] _noaa_ops.h5	IDPS outputs of SDR data	HDF5
	3	GONPO_npp_IDP STime [§] _noaa_ops.h5	IDPS outputs of GEO data	HDF5
	4	SOMTC_npp_IDP STime [§] _noaa_ops.h5	IDPS outputs of SDR data for OMPS NM	HDF5
	5	GOTCO_npp_IDP STime [§] _noaa_ops.h5	IDPS outputs of GEO data for OMPS NM	HDF5
Ancillary File	6	band_centers.txt	Wavelengths and assumed bandpass	ASCII

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			FWHM for each measurement channel	
	7	cloud_ground_pres sure.nc	Cloud pressure data	netCDF
	8	mrgapprf.dat	Merged a priori ozone climatology	ASCII
	9	O3_CLIM13.DAT	A priori ozone profile climatology	ASCII
	10	profile_dndx.nc	Profile N-value sensitivity look-up table	netCDF
	11	profile_table.nc	Profile N-value look-up table	netCDF
	12	solar_bass.dat	Solar radiation reference look-up table	ASCII
	13	TM_CLIM13.DAT	A priori temperature profile climatology	ASCII
	14	v8std81.dat	Standard profiles in fine layers	ASCII

[§]IDPSTime=dyyyymndd_thhmmss0_ ehhmmss0_b21447_cyyyymnddhhmmssxxxxx, where the first character d, t, e, b, c, indicate the date, starting time, ending time, orbital number, creation time, and yyyy, mn, dd indicate the year, month, and day, while hh and the second mm, indicate the hour, minute. The ss0 and ssxxxxx give tenths of seconds and microseconds respectively.

PERFORMANCE

Product Testing

Test Data

Description of all NDEV8P test data (input, output) used in unit and system tests is provided in the NDE V8Pro Algorithm Readiness Review Report (NESDIS/STAR, 2016). This is available by contacting the Product Area Lead (PAL) at OSPO.

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Test Plans

Description of all NDEV8P test plans used in unit and system tests is provided in the NDE V8Pro Algorithm Readiness Review Report (NESDIS/STAR, 2016). These are available by contacting the Product Area Lead (PAL) at OSPO.

Product Accuracy

Test Results

Description of all NDEV8P test results from the unit and system tests are provided in the NDE V8Pro Algorithm Readiness Review Report (NESDIS/STAR, 2016). This is available by contacting the Product Area Lead (PAL) at OSPO.

Product Accuracy

The V8Pro products have been made offline for the first four years of the OMPS NP mission. Results and products have been tracked at the STAR ICVS system at http://www.star.nesdis.noaa.gov/smcd/spb/OMPSDemo/proOMPSbeta.php

Product accuracy estimates can also be made by using the performance of the heritage SBUV/2 products.

Product Quality

The Error Flags listed in Table 1-4 gives the decoding for the various error flag results. Intermediate products within the output EDR can also be used to check for unusual conditions.

Analysis Tools

No external product tools are supplied. The NDEV8P output files are netCDF4 files. External users can choose their own tools to display and analyze these output files. BUFR Versions of selected content are under development.

PRODUCT STATUS

Operations Documentation

Operational logs contain the information regarding the changes made to science, instruments, and systems. Basically the Configuration Management system will have the

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detailed information about these changes, but operational logs keep the high level description of these changes.

NESDIS/STAR (2015), Version 8 Ozone Algorithm Theoretical Basis Document.

NESDIS/STAR (2016), NDE Version 8 Ozone Profile Maintenance Manual, Version 1.0.

NESDIS/STAR (2016), NDE Version 8 Ozone Profile Algorithm Readiness Review Report (ARRR)

NDE Operations Handbook Version 1.0 (2013)

Maintenance History

The System Maintenance Manual (SMM) will be updated to reflect the changes that will be required to maintain the **NDE Version 8 Ozone Profile** system within the ESPC environment. Information regarding the changes to the products is tracked by the Operational logs and will be available to users on request. Product metadata will be updated as per the changes required in the product including the version number, quality flags etc.

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Mateer, C.L., D.F. Heath, & A.J. Krueger, "Estimation of total ozone from satellite measurements of backscattered ultraviolet Earth radiance," *J. Atmos. Sci.*, **28**, 1307-1311, 1971.

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END OF DOCUMENT