NOAA NESDIS
CENTER for SATELLITE APPLICATIONS and RESEARCH

The NOAA Suomi-NPP Data Exploitation (NDE) Version 8 Total Ozone (V8TOz) Environmental Data Record (EDR) NDEV8T

External Users' Manual

Version 1.1

TITLE: NDE VERSION 8 TOTAL OZONE 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.

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LIST OF CHANGES

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

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LIST OF CHANGE-AFFECTED PAGES/SECTIONS/APPENDICES					
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1.0	03/10/16	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 Total Column Ozone Environmental Data Record product and output file. The NDEV8T provides the Ozone Mapping and Profiler (OMPS) Total Column Ozone bundled product as created by the Version 8 Total Ozone 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 NDEAF processing, but available only internally within the NDE.

Product Overview

Product Requirements

All NDEV8TOz basic and derived requirements are available in the NDEAF 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 Total Column Ozone EDRs from the JPSS program.

Product Team

The NDEV8T 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.

Table 1-1 Product Team Members

Team Member	Organization	Role	Contact Information
Lawrence Flynn	STAR	STAR Product Lead	5830 University Research Court Riverdale, MD. 20740 Phone: 301-683-3612 Email: Lawrence.E.Flynn@noaa.gov
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Product Description

The NDEV8T product was developed to generate Total Colum Ozone estimates from a discrete set of 12 measurements of backscattered ultraviolet radiances in the 308 nm to 380 nm range. In addition to the total ozone estimates, it produces effect 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 Mapper Sensor Data Records (SDRs) pixels globally. Details on the content of the NDEV8T external output files are provided in section 1.3.

Product History

The NDEV8T is a new implementation of the Version 8 Total Column Ozone developed by NASA GSFC for the Total Ozone Mapping Spectrometer (TOMS) 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 EUMETSAT Global Ozone Monitoring Experiment (GOME-2) instruments. This product replaces the current operational IDPS Total Column Ozone IP an EDR products (INCTO and OOTCO). The IDPS product meets the JPSS Level 1 requirements with the exclusions applicable for Suomi-NPP only. The new product will couple with the Linear Fit SO2 algorithm to provide corrections to the total column ozone estimates for elevated atmospheric SO2 amounts. It will also be consistent with the existing NOAA GOME-2 and NASA TOMS/OMI records.

Product Access

All NDEV8T 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 NDEV8T (i.e., the Atmospheric Chemistry) 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 needs to fill out the Data Access Request Form located on http://www.ospo.noaa.gov/Organization/About/access.html and submits to the PAL with a copy to nesdis.data.access@noaa.gov. CLASS will be archiving the NDEAF 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 NDEAF product in netCDF4 format with associated metadata.

Table 1-2 describes the external distributed NDEV8T file and Table 1-3 lists its content. Details of the derivation of all of the products are described in the NDE Version 8 Total Ozone Algorithm Theoretical Basis Document.

Table 1-3 describes the variables in file. The ozone total column is defined as the amount of Ozone in a vertical column of the atmosphere measured in Dobson Units (1 DU = 1 milli-atm-cm). The key EDR product is the ColumnAmountO3 estimate.

Table 2-2 NDE Total Column Ozone File

File	Description	Format	Size/file
V8TOZ-EDR_v1r0_npp_s201601120127494_e201601120128268_c20160322150300 0.nc	This is the granule output file containing all the derived variables of the NDEV8T product.	netCDF4	0.9 MB/granule file, ~1009 files/day

Table 3-3 Total Column Ozone Output Granule File Content

Name	Type	Description	Dimension	Units	Range
Latitude	32 bit Float	Latitude	15 x 105	Degrees	-90 ~ 90
Longitude	32 bit Float	Longitude	15 x 105	Degrees	-180 ~ 180
SolarZenithAngle	32 bit Float	Solar Zenith Angle	15 x 105	Degrees	0 ~ 180
SatelliteViewAngle	32 bit Float	Satellite View Angle	15 x 105	Degrees	-90~ 90
RelativeAzimuth	32 bit Float	Relative Azimuth	15 x 105	Degrees	-180~ 180
AerosolIndex	32 bit Float	Aerosol Index	15 x 105	Unitless	-100~ 100
AlgorithmFlag	32 bit Integer	Algorithm Flag	15 x 105	Unitless	0 ~ 10
CloudFraction	32 bit Float	Cloud Fraction	15 x 105	Unitless	0~ 1
CloudTopPressure	32 bit Float	Pressure at top of cloud	15 x 105	hPa	10~ 2000
ColumnAmountO3	32 bit Float	V8TOZ Total Column of Ozone	15 x 105	Dobson Units	0~ 1000
EclipseFlag	32 bit	Eclipse Flag	15 x 105	Unitless	0~ 10

	Float				
ErrorFlag	32 bit Integer	Error Flag	15 x 105	Unitless	0~ 10
O3BelowCloud	32 bit Float	Total Column of Ozone below Cloud	15 x 105	Dobson Units	0~ 1000
QualityFlag	32 bit Integer	Quality Flag	15 x 105	Unitless	0~ 10
Reflectivity331	32 bit Float	Average 331 nm Reflectivity from V8TOz retrieval	15 x 105	%	0~ 100
Reflectivity360	32 bit Float	Average 360 nm Reflectivity from V8TOz retrieval	15 x 105	%	0~ 100
So2Index	32 bit Float	So2 Index	15 x 105	Unitless	-100~ 100
Step1Ozone	32 bit Float	V8TOZ Step1 Ozone	15 x 105	Dobson Units	0~ 1000
Step2Ozone	32 bit Float	V8TOZ Step2 Ozone	15 x 105	Dobson Units	0~ 1000
SunGlintFlag	32 bit Float	Sun Glint Flag	15 x 105	Unitless	0~ 10
NvalueAdjustment	32 bit Float	N-Value adjustment for 12 V8TOZ wavelengths	105 x 12	N-Values	-20~ 20
NvalueMeasured	32 bit Float	V8TOz Measured normalized radiances for 12 V8TOZ wavelengths	15 x 105 x 12	N-Values	0~ 100
Step1Residual	32 bit Float	V8TOZ Step 1 Residuals	15 x 105 x 12	N-Values	-50~ 50
Step2Residual	32 bit Float	V8TOZ Step 2 Residuals	15 x 105 x 12	N-Values	-50~ 50
Step3Residual	32 bit Float	V8TOZ Step 3 Residuals	15 x 105 x 12	N-Values	-50~ 50
dNdOmega	32 bit Float	V8TOz ozone sensitivities	15 x 105 x 12	N-Value/Dobson unit	-20~ 50

dNdR	32 bit Float	V8TOz reflectivity sensitivities	15 x 105 x 12	N-Values	0~ 600
LayerEfficiency	32 bit Float	V8TOz Layer retrieval efficiencies	15 x 105 x 11	DU/DU	-1~ 10
TemperatureProfile	32 bit Float	Temperature Profile	15 x 105 x 11	Degrees Kelvin	100~ 400
Step2Profile	32 bit Float	Step2 Ozone Profile	15 x 105 x 11	Dobson Units	10~ 400
TerrPressure	32 bit Float	Terrain Pressure from LUT	15 x 105	hPa	100~ 1500
Wavelengths	32 bit Float	12 Wavelengths of Observation for V8TOz	12	nm	300~ 420
ScanTime	62 bit Float	Elapsed time in seconds since Jan 1, 1958 including leap seconds	15	Microseconds	1.0~ 1.0E12
Ascending_Descending	32 bit Integer	1=Descending, 0=Ascending	15	Unitless	0~ 1
quality_information	8 bit Character	Granule quality information	1	%	0.0~ 100.0
38 V8TOZ diagnostic variables	See netCDF4 metadata	Variables to describe observing and environmental conditions, and results of algorithm tests	38	See netCDF4 metadata	See netCDF4 metadata

Table 1-4 decodes the total ozone error flag values.

Table 4-4 Details of the Error Flag

Output	Type	Description	
ErrorFlag	16-bit signed integer	Good – 0	Good retrieval SZA <= 84º
		Glint – 1	Open water with sun glint geometry present
		SZA - 2	Good retrieval SZA > 84º
		Aerosol – 3	360 nm residual > threshold
		Shape – 4	Residual at unused ozone wavelength > 4 σ
		SO2 – 5	S)2 Index > 4 σ
		NC – 6	Algorithm does not converge
		Residual – 7	Absolute residual > 32
		+10	Add 10 for Descending Orbit data

ALGORITHM

Algorithm Overview

The NDEV8 product is generated from the Version 8 Total O_3 algorithm (V8TOz) .The Version 8 total O_3 algorithm (V8TOZ) is the most recent version of a series of BUV (backscattered ultraviolet) total O_3 algorithms that have been developed since the original algorithm proposed by *Dave* & *Mateer* [*1967*], which was used to process Nimbus-4 BUV data [*Mateer* et al., *1971*]. The algorithm makes two key assumptions about the nature of the BUV radiation. Firstly, we assume that the BUV radiances at wavelengths greater than 310 nm are primarily a function of total O_3 amount, with only a weak dependence on O_3 profile that can be accounted for using a set of standard profiles. Secondly, we assume that a relatively simple radiative transfer model that treats clouds, aerosols, and surfaces as Lambertian reflectors can account for most of the spectral dependence of BUV radiation, though corrections are required to handle special situations. The algorithm uses measurements at 12 channels to esitmate the effective reflectivty and createabsorbing aerosol and SO2 indices. A radiative transfer lookup table created using standard ozone profiiles is used to match the viewing conditions and an ozone absorbing channel

measurement.The Vesrin 8 algorithm has incorporated procedures for identifying the special situations, and apply semi-empirical corrections, based on accurate radiative transfer models, to minimize the errors that occur in these situations. The following sections describe the input files.

Input Satellite Data

Satellite Instruments

NDEV8T is a system operated within the NDE DHS by OSPO. It uses measurements from the Ozone Mapping and Profiler Suite (OMPS) 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 1:30pm 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 105º 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 current operated to aggregate approximately 20 spatial pixels into 35 cross-track bin and to integrate for approximately 7.8 S. This produces 50x50 km^2 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 km^2 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 12 wavelengths for the V8TOz EDR algorithm are obtained by interpolating the values at adjacent measurement wavelengths to provide them at the following 12 wavelengths:

[308.7,310.8,311.9,312.61,313.2,314.4, 317.6,322.4,331.3,345.4,360.2,372.8] nm

Satellite Data Preprocessing Overview

The OMPS Raw Data Records (RDRs) are processed at IDPS into Sensor Data Records (SDRs) by the 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 NDEV8T algorithm uses the radiance and irradiance measurements provide in the OMPS NM SDR and the geolocation and viewing geometry information provided in the OMPS NM GEO. Table 2-1 provides a summary of the OMPS SDR and GEO parameters used by the algorithm.

Table 2-1 OMPS SDR and GEO data used by the NDEV8T algorithm

Input	Type	Description	Units/Valid Range
Pixel-Level Data Items			
satza	real	Satellite zenith angle	Degrees
sza	real	Solar zenith angle	Degrees
xphi	real	Relative azimuth angle between sensor and solar azimuth angles	Degrees
month	integer	Month of measurement	Month / 1 – 12
day	integer	Day of month of measurement	Day
seconds	long interger	Seconds in day of mesurment	Seconds
xlat	real	Latitude of measurement	Degrees / -90 – 90
xlong	real	Longitude of measurement	Degrees / -180 – 180
xm	real	Radiances for 24 sensor wavelengths	W/m^2-nm / 0 – $3x10^7$
Sflux	real	Solar flux for 24 sensor wavelengths	W/m^2-nm / 0 – $3x10^7$

Input Ancillary Data – Climatolgy and RT LUTs.

The NDEV8T 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 Climatological and Table data used by the NDEV8T algorithm

Input	Type	Description	Units/Valid Range
Pixel-Level Data Items			
Wl0	real	12 sensor wavelengths to use for measurement	nm / 290 – 390
pcloud	real	Cloud top pressure climatology	hPa / 0 – 1013.25
pteran	real	Terrain pressure climatology	hPa / 0 – 1013.25
prftemp	real	Temperature profile climatology for 11 Umkehr layers	Degrees Kelvin (K) / 170 – 350
isnow	integer	Snow/ice flag	Unitless / 0 – 1
prfoz	real	TOMS V8 Ozone Profile Climatology Data for 11 Umkehr layers	DU / 0 – 999 (0 – 200 for non-fill)
cwavl	real	Wavelength for absorption coefficient	nm / 290 – 390
c0	real	Absorption coefficient at cwavl at 273 K	atm / cm / 0 – 5
c1	real	Linear temperature correction Coefficient to c0	atm / cm / K / 0 - 0.08
c2	real	Quadratic temperature correction Coefficient to c0	atm / cm / K^2 /-0.002 to 0.002
o3abs	real	Ozone absorption coefficients used in SOI algorithm	atm / cm /
logi0,z1, z2, tr, knb, sb	real	OMPS V8TOz LUT values	
logi0_dndx, z1_dndx , z2_dndx , tr_dndx , knb_dndx , sb_dndx	real	OMPS V8TOz Sensitivity LUT values	

PERFORMANCE

Product Testing

Test Data

Description of all NDEV8T test data (input, output) used in unit and system tests is provided in the NDE V8TOz Algorithm Readiness Review Report (NESDIS/STAR, 2016). This is available by contacting the Atmospheric Chemistry Area Lead (PAL) at OSPO.

Test Plans

Description of all NDEV8T test plans used in unit and system tests is provided in the NDE V8TOz Algorithm Readiness Review Report (NESDIS/STAR, 2016). These are available by contacting the Atmospheric Chemistry Area Lead (PAL) at OSPO.

Product Accuracy

Test Results

Description of all NDEV8T test results from the unit and system tests is provided in the NDE V8TOz Algorithm Readiness Review Report (NESDIS/STAR, 2016). This is available by contacting the Atmospheric Chemistry Area Lead (PAL) at OSPO.

Product Accuracy

The V8TOz products have been made off line for the first three years of the OMPS NM 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 be also be made for the performance of the heritage OMI products.

Product Quality

The ErrorFlag listed in listed 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 NDEV8T 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 detailed information about these changes, but operational logs keep the high level description of these changes.

NESDIS/STAR (2015), NDE Version 8 Total Column Ozone Algorithm Theoretical Basis Document, Version 1.0.

NESDIS/STAR (2015), NDE Version 8 Total Column Ozone Maintenance Manual, Version 1.0.

NESDIS/STAR (2015), NDE Version 8 Total Column Ozone 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 Total Ozone** 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.

REFERENCES

Dave, J.V. & C.L. Mateer, "A preliminary study on the possibility of estimating total atmospheric ozone from satellite measurements," *J. Atmos. Sci.*, **24**, 414-427, 1967.

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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