Satellite Products and Services Review Board

# Algorithm Theoretical Basis Document for NOAA NDE OMPS Version 8 Ozone Profile (V8PRO) Environmental Data Record (EDR) Version 1.0



TITLE: FOR NOAA NDE OMPS VERSION 8 OZONE PROFILE

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Remarks: This document shares algorithm descriptive material with the corresponding NASAsponsored Version 8 Ozone Profile algorithm theoretical basis document.

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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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#### 1. INTRODUCTION

This document presents the scientific background, design and performance of the Ozone Mapping and Profiler Suite Nadir Profier (OMPS NP) Version 8 Ozone Profile (V8PRO) Environmental Data Record (EDR) algorithm for the Joint Polar Satellite System (JPSS). The V8PRO algorithm produces a bundled set of outputs from OMPS NP and OMPS Nadir Mapper (NM) measurements..

Products from the OMPS V8PRO algorithm described here fulfill the requirements identified in the JPSS OMPS Ozone Profile. Furthermore, those requirements provide continuity to the NASA EOS Aura Ozone Monitoring Instrument (OMI).

#### 1.1. Product Overview

#### **1.1.1. Product Description**

Product description with sufficient detail so that the user understands how to use the product files. (Document Object 34)<sup>1</sup> Writers: Algorithm Scientists.

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.

#### **1.1.2. 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.

#### **1.1.3. Product Requirements**

State the requirements for each product, either explicitly or by reference to the project's requirements document, if available. Product requirements should include content, format, latency, quality. (Document Object 1)

#### Writers: Development Lead.

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.

#### **1.2. Satellite Instrument Description**

Describe the attributes of the sensing system(s) used to supply data for the retrieval algorithm at a level of detail sufficient for reviewers to verify that the instrument is capable of supplying input data of sufficient quality. (Document Object 28)
<u>Writers:</u> Development Lead and PAL should collaborate.
(Document Object 28)

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 km<sup>2</sup> 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<sup>2</sup> 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:

[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 ??

#### 2. ALGORITHM DESCRIPTION

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.

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 O<sub>3</sub> profile retrievals which now use the same set of *a prioris*). The V8PRO has improved total O<sub>3</sub> 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.

#### 2.1. Processing Outline

Full description of the processing outline of the retrieval algorithm. All key elements and subelements needed to convey a comprehensive sense of the algorithm should be included. The level of detail should be consistent with the current maturity of the software architecture (which will improve with each revision). A data flow diagram consistent with the software architecture is preferred. (Document Object 13) Writers: Algorithm Scientists.

The OMPS V8PRO is a self-contained algorithm with no dependencies on other Level 2 products. It reads input OMPS Sensor Data Record (SDR) and Geolocation Data Records (GEO) from both the NM and NP sensors and combines these with climatological and radiative transfer lookup table (RTLUT) input to generate the Ozone profile estimates. All OMPS Earth View SDRs on the dayside of the orbit are processed individually.

#### **Description modules of NDE-V8PRO algorithm:**

Main program: O3P\_main.f90

Here is the description of all the routines used in this package.

#### Subroutine altitude (altitude.f90)

Subroutine altitude is a subroutine to compute the geophysical altitude based on temperature and pressure. It calculates physical heights at specified pressure levels. Called by o3\_retrieval and profile.

#### Subroutine aprsbo (stndprof.f90)

Subroutine to read in a priori ozone. Called by total.

#### Subroutine aprsbt (stndprof.f90)

Subroutine to read in a priori temperature. Called by total.

#### Subroutine blwcld (blwcld.f90)

Subroutine blwcld is a subroutine to estimate the amount of ozone below a cloud pressure level using standard ozone profile climatology. Called by total.

#### Subroutine cnstnts (start.f90)

Subroutine for initializing various constant parameters used in the retrieval. Called by start. Calls coffs.

#### coffs (start.f90)

Subroutine for assigning optical coefficients and weights for SBUV sub-channels. Called by cnstnts.

#### Module constants (constants.f90)

Module constants is a model that sets parameters for total ozone retrievals.

#### Module control (control.f90)

Module control is a module that has indexing parameters to set which measurement values to use from the input nvalue.

#### Subroutine copy\_geoloc\_to\_output (geo\_mod.f90)

Subroutine copy\_geoloc\_to\_output is a subroutine to place geolocation data into the output. Called by scanin.

#### Subroutine convert20 (profile\_datamod.f90)

Subroutine convert20 is a subroutine to convert 80 layer profiles to 20 layer ones. Called by profile.

#### Subroutine data\_ingest (data\_ingest.f90)

Subroutine data\_ingest is a subroutine to prepare and ingest all necessary data to process version 8 ozone profile retrieval algorithm.

Calls init\_netcdf, fillval\_retrieval\_fields, total, profile, write\_global\_output, total\_to\_netcdf, profile\_to\_netcdf.

Called by O3\_main.

#### Subroutine dn\_by\_dt (dndt.f90)

Subroutines for computing the change in N-value due to temperature difference for each of 11 Umkehr layers and each of 8 wavelengths using a chain rule relating dN / dT to dN / dX. Subroutine dndt is a module to handle calculation of the temperature correction at the standard pressure layers.

Called by total and msr\_temp\_adjust.

#### Subroutine factor (linsolve.f90)

Subroutine factor is a subroutine for performing an LU factorization of a general matrix of dimension N x N.

Called by update and convert20.

#### Subroutine fillval\_retrieval\_fields (output.f90)

Subroutine fillval\_retrieval\_fields is a subroutine for setting retrieved quantities to zero, initial values.

Called by data\_ingest.

#### Module geo\_mod (geo\_mod.f90)

Module geo\_mod is a Module to track the geolocation and viewing geometry of the observation. Module to store ground pixel level information such as snow ice, cloud pressure, and measurement geometry.

#### Subroutine getmsr (getmsr.f90)

Subroutine getmsr is a subroutine to compute nvalues from radiative transfer tables specific to the version 8 total ozone channel. It computes the multiple scattered and surface reflected part of the Jacobian for each of 11 Umkehr layers and each of 8 wavelengths by using finite differencing between N-values interpolated from unperturbed and perturbed ozone tables. 12 tables are contained in common: 1 unperturbed followed by 11 with perturbations in Umkehr layers 0–9 and the sum of layers 10-12.

Calls getmsr\_single\_chan. Called by total.

#### Function getfilename (O3P\_input\_class.f90)

Function getfilename is for reading in file names from control file. Called by O3P\_main.

#### Subroutine getrng (getrng.f90)

Subroutine getrng is a subroutine for interpolating appropriate ring effect corrections in reflectivity and pressure. This is the RRS (Rotational Raman Scattering) correction. This corrects for inelastic scattering in the atmosphere from molecular oxygen and nitrogen. Called by reflec and residue.

#### Subroutine getshape (getshape.f90)

Subroutine getshape is a subroutine to compute an ozone apriori profile from climatology based on total ozone, day of year and latitude. Called by total.

#### Subroutine init\_dndt (dndt.f90)

Subroutine init\_dndt.f90 is a subroutine to initialize ozone absorption coefficients for profile channels.

Called by start.

#### Subroutine init\_dndt\_toz (dndt.f90)

Subroutine init\_dndt\_toz is a subroutine to initialize ozone absorption coefficients for total ozone channels.

Called by start.

#### Subroutine init\_netcdf (netcdf\_util.f90)

Subroutine init\_netcdf is a subroutine to declare dimensions and variables for writing out data in NetCDF format .

Called by data\_ingest.

#### Subroutine init\_retrieval (init\_retrieval.f90)

Subroutine init\_retrieval.f90 is a subroutine that performs initial input of v8pro required ancillary data. Calls start. Called by O3P\_main.

#### Subroutine inter (inter.f90)

Subroutine inter is a module to interpolate climatological values of snow ice, surface type, and cloud pressure. The subroutine within it are run to find terrain, cloud pressure, snow/ice, and surface category code from appropriate data bases for a given date, latitude and longitude. Called by scanin.

Calls insurf and incovr.

#### Subroutine interp\_dndx (msr.f90)

Subroutine interp\_dndx is a subroutine to interpolate table entries. Called by getmsr\_single\_chan and msr\_component.

#### Subroutine interp\_rad (msr.f90)

Subroutine interp\_rad is a subroutine to interpolate table entries in pressure. Called by rad msr and iztrsb.

Calls interp\_sza\_vza.

#### Subroutine interp\_sza\_vza (msr.f90)

Subroutine interp\_sza\_vza is a subroutine to interpolate table entries in solar and viewing angles.

Called by interp\_rad.

#### Subroutine interpol\_kern (interpol\_kern.f90)

Subroutine interpol\_kern is a subroutine to interpolate a multiple scattering kernel to a finer pressure level. Called by profile.

#### Subroutine interpol\_qo3 (interpol\_qo3.f90)

Subroutine interpol\_qo3 is a subroutine to convert a 21 layer ozone profile into 81 layers on a finer pressure grid. Calls splinev8. Called by profile.

#### Subroutine interpol\_t (interpol\_t.f90)

Subroutine interpol\_t uses splines to convert a 21 layer climatological temperature profile to the 81 layer temperature profile used in the ozone profile retrieval. Calls splinev8. Called by profile.

#### Subroutine inverse (linsolve.f90)

Subroutine inverse inverts a matrix. Called by o3\_retrieval, convert20, and update.

#### Subroutine iztrsb (iztrsb.f90)

Subroutine iztrsb is a subroutine to compute components of the nvalue calculation from radiative transfer tables. It performs interpolations of the table parameters 0 *i*, *r T*, and *b s*, which are used by thecalling routines to calculate table radiances or N-values. It uses Lagrangian interpolation except for high clouds for which a linear extrapolation is used. Called by oznot, refl\_360, reflec, and residue. Calls interp\_rad.

#### Subroutine linear\_fit (linear\_fit.f90)

Subroutine linear\_fit is a subroutine to do a linear least squares fit of a set of points. Called by o3\_retrieval.

#### Module Ipoly (Ipoly.f90)

Module lpoly is a module to define lagrangian interpolation coefficients. Used in interp\_dndx, interp\_sza\_vza, , scanin, and cnstnts.

#### Subroutine mixratio (mixratio.f90)

Subroutine mixratio is a subroutine to compute the volume mixing ratio estimated ozone profile using the current estimated ozone in DU (Dobson Unit). It determines ozone mixing ratio and its estimated percentage error at prescribed pressure levels. Called by profile. Calls splinev8.

#### Module msr (msr.f90)

Module msr is a module that has subroutines to compute nvalues from radiative transfer tables.

#### Module msr\_temp\_adjust (msr.f90)

Subroutine msr\_temp\_adjust is a subroutine to compute adjustments for temperature differences.

Calls dn\_by\_dt. Called by total.

#### Subroutine nvbrac (oznot.f90)

Subroutine nvbrac.f90 is a subroutine to perform N-value bracketing and prepare for interpolation.

Called by oznot.

#### Subroutine o3\_retrieval (o3\_retrieval.f90)

Subroutine o3\_retrieval is a subroutine to carry out the version 8 ozone retrieval using maximum likelihood estimation. It performs ozone retrievals by using Rodgers method. Calls linear\_fit, altitude, o3\_snglscatt, update and inverse. Called by profile.

#### Subroutine o3\_snglscatt (o3\_snglscatt.f90)

Subroutine o3\_snglscatt is a subroutine that is the primary single scatter radiative transfer calculator. It computes the ozone single scattering approximation. Called by o3\_retrieval.

#### module O3P\_input\_class (O3P\_input\_class.f90)

Module O3P\_input\_class Contains the functions that read in the namelist from control file (getFileName) and read in geo/sdr data from IDPS outputs , and makes module O3T\_input\_class.mod.

Calls getfilename, rd\_gotco, rd\_somtc, rd\_somps and rd\_gonpo. Called by O3P\_main.

#### program O3P\_main (O3P\_main.f90)

Program O3P\_main is the main program that reads in control file which contains all input file (SDR and ancillary data) needed for processing v8profile algorithm. The program performs searching and averaging TC data within NP FOV, and makes interpolation of earth radiance and solar flux into target wavelengths that used in the V8PRO retrieval. The program also acts as an interface to the v8profile retrieval code.

Calls init\_retrieval, data\_indest.

#### Subroutine oznot (oznot.f90)

Subroutine oznot is a subroutine to compute initial ozone estimate using the 317.5 nm channel.

Called by total.

Calls iztrsb, getrngand nvbrac.

#### Subroutine ozone (ozone.f90)

Subroutine ozone is a subroutine to compute step3 ozone or best ozone for the total ozone algorithm.

Called by total.

#### Module output (output.f90)

Module output is a module that stores values for output.

#### Function pintrp (pterp.f90)

Function pintrp is a function to set up pressures for interpolation.

#### Subroutine prfind (reflec.f90)

Subroutine prfind finds table entries for reflectivity computations. Called by reflec.

#### Module pterp (pterp.f90)

Module pterp is a module to interpolate in pressure using lagrangian interplation method.

#### Module press\_interp (msr.f90)

Function press\_interp is a function to interpolate in pressure using lagrangian interpolation. Called in interp\_rad.

#### Subroutine profile (profile.f90)

Subroutine profile is a high level subroutine that does the ozone profile estimation. This is the subdriver for profile ozone retrieval.

Calls Interpol\_qo3, Interpol\_t, Interpol\_kern, o3\_retrieval, set\_profile\_output, convert20, mixratio, altitude, and splinev8.

Called by data\_ingest.

#### Module profile\_data\_module (profile\_datamod.f90)

Module profile\_data\_module is a module that stores input data to the ozone profile estimation algorithm.

#### Subroutine profile\_to\_netcdf (netcdf\_util.f90)

Subroutine profile\_to\_netcdf is a subroutine to write profile ozone calculation results for NetCDF formatted output file. Called by data\_ingest.

#### Subroutine rad\_msr (msr.f90)

Subroutine rad\_msr is a subroutine to perform N-value table computations. Calls interp\_rad. Called by total.

#### Subroutine rdcons (constants.f90)

Subroutine rdcons is in constants.f90. It is a subroutine that stores constants used in the Version 8 retrieval. It reads in instrument dependent constants. Called by start. Calls set\_best\_ozone\_chans.

#### Subroutine RD\_GOTCO (O3P\_input\_class.f90)

Subroutine RD\_GOTCO is a subroutine that reads in HDF formatted NM GEO file. Called by O3\_main.

#### Subroutine RD\_GONPO (O3P\_input\_class.f90)

Subroutine RD\_GONPO is a subroutine that reads in HDF formatted NP GEO file. Called by O3\_main.

#### Subroutine RD\_SOMTC (O3P\_input\_class.f90)

Subroutine RD\_SOMTC is a subroutine that reads in HDF formatted NM SDR file. Called by O3\_main.

#### Subroutine RD\_SOMPS (O3P\_input\_class.f90)

Subroutine RD\_SOMPS is a subroutine that reads in HDF formatted NP SDR file. Called by O3\_main.

#### Subroutine read\_clim (stndprof.f90)

Subroutine read\_clim is a subroutine to read in climatological profiles. Called by start.

#### Subroutine read\_instrument\_table (msr.f90)

Subroutine read\_instrument table is a subroutine to read in instrument tables. Called by read\_msr\_tables.

#### Subroutine read\_instrument\_dndx (msr.f90)

Subroutine read\_instrument\_dndx is a subroutine to read in instrument sensitivity tables. Called by read\_msr\_tables.

#### Subroutine read\_msr\_tables (msr.f90)

Subroutine read\_msr\_tables is a subroutine to read in multiple scattering tables. Called by start.

Calls read\_instrument\_table and read\_instrument\_dndx.

#### Subroutine reflec (reflec.f90)

Subroutine reflecv8 is a subroutine to compute reflectivity values using measured nvalue and computed nvalue. Calls prfind, iztrsb and getrng. Called by total.

#### Subroutine refl\_360 (refl\_360.f90)

Subroutine refl\_360 is a subroutine to compute the reflectivity at the longest wavelength measurement. Calls iztrsb. Called by total.

#### Subroutine resadj (resadj.f90)

Subroutine resadj is a subroutine that adjusts total ozone residual values from dndx values after calculation of best ozone. Called by total.

#### Subroutine residue (residue.f90)

Subroutine residue is a subroutine to compute the difference between a computed nvalue and measured nvalue. It computes the residues for each of the multiple scattered wavelengths. Calls residue\_single\_chan. Called by total.

#### Subroutine residue\_single\_chan (residue.f90)

Subroutine residue\_single\_chan is a subroutine to compute residuals for single channels. Calls iztrsb and getrng. Called by residue.

#### Subroutine scanin (scanin.f90)

Subroutine scanin is a counterpart to the v6 scanin subroutine. It sets internal parameters based on solar zenith angle and surface pressure. Calls inter and copy\_geoloc\_to\_output. Called by total.

#### Subroutine set\_best\_ozone\_chans (control.f90)

Subroutine to set the ozone channels. Called by rdcons.

#### Subroutine seterr (seterr.f90)

Subroutine seterr is a subroutine to set error flags for the version 8 total ozone algorithm. Subroutine for setting error flags. Called by total.

#### Subroutine set\_profile\_output (profile.f90)

Subroutine set\_profile\_output is a subroutine to load profile ozone variables for a scan. Calls altitude and splinev8. Called by profile.

#### Subroutine set\_total (total.f90)

Subroutine set\_total is a subroutine to load total ozone variables for a scan. Called by total.

#### Subroutine splinev8 (splinev8.f90)

Subroutine splinev8 is a subroutine to perform clamped cubic spline implementation. Called by interpol\_qo3, interpol\_t, mixratio, and profile.

#### Subroutine start (start.f90)

Subroutine start is a subroutine to initialize startup values for the version 8 retrieval. Calls read\_clim, rdcons, cnstnts, read\_msr\_tables, init\_dndt, and init\_dndt\_toz. Called by init\_retrieval.

#### Module stndprof (stndprof.f90)

Module stndprof is a module that provides subroutines (aprsbo, aprsbt, and read\_clim) to interpolate standard ozone profiles to determine a priori ozone profile for a given day and latitude.

#### Subroutine stnp81 (stnp81.f90)

Subroutine stnp81 is a subroutine to determine a standard profile associated with a specific total ozone value and a single latitude band. Called by total.

#### Subroutine total (total.f90)

Subroutine total is a subroutine that carries out the high level management of the total ozone retrieval. It is the driver for processing one scan of data from the level 1 SBUV record and computing the total ozone used as first guess in the profiling algorithm. Calls scaninv8, reflecv8, refl\_360, oznot, residue, rad\_msr, getmsr, msr\_component, aprsbo, aprsbt, stnp81, dn\_by\_dt, resadj, msr\_temp\_adjust,

getshape, ozone, resadj, blwcld, seterr and set\_total\_output. Called by data\_ingest.

#### Subroutine total\_to\_netcdf (netcdf\_util.f90)

Subroutine total\_to\_netcdf is a subroutine to write total ozone calculation results for NetCDF formatted output file.

Called by data\_ingest.

#### Module totret (totret.f90)

Module totret is a module to store data values for the v8pro total ozone algorithm.

#### Subroutine update (update.f90)

Subroutine update is a subroutine to carry out maximum likelihood estimation computations. It updates the ozone profile using C. Rodgers' method. Calls factor and inverse. Called by o3\_retrieval.

#### Subroutine write\_global\_output (netcdf\_util.f90)

Subroutine write\_global\_output is a subroutine to write global variables and attributes for NetCDF formatted output file. Called by data\_ingest.

**FLOW CHARTS FOR V8PRO** 









Figure 2.1: The Flow Charts (Chart 1, Chart 2, Chart 3 and Chart 4)

#### The modules for NDE-V8PRO algorithm:

The OMPS NP V8 main source code consists of 13,108 lines in 45 files. It is written in FORTRAN 90 language.

The routines are: altitude.f90 blwcld.f90 constants.f90 data\_ingest.f90 dndt.f90 geo\_mod.f90 getmsr.f90 getrng.f90 getshape.f90 init retrieval.f90 inter.f90 interpol kern.f90 interpol\_qo3.f90 interpol t.f90 iztrsb.f90 linear fit.f90 linsolve.f90 lpoly.f90 mixratio.f90 msr.f90 netcdf\_util.f90 O3P\_input\_class.f90 O3P\_main.f90 o3 retrieval.f90 o3\_snglscatt.f90 output.f90 oznot.f90 ozone.f90 profile\_datamod.f90 profile.f90 pterp.f90 refl 360.f90 reflec.f90 resadi.f90 residue.f90 scanin.f90 seterr.f90 splinev8.f90 start.f90 stndprof.f90 stnp81.f90 total.f90 totret.f90 update.f90

#### 2.2. Algorithm Input

Full description of the attributes of all input data used by the algorithm, including primary sensor data, ancillary data, forward models (e.g. radiative transfer models, optical models, or other model that relates sensor observables to geophysical phenomena) and look-up tables. Do not include file formats; these will be documented elsewhere. *(Document Object 14)* **Writers:** Algorithm Scientists.

#### 2.2.1. Input Satellite Data

#### 2.2.2. 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 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. OMPS NP EDR algorithm also requires OMPS NM SDR and geolocation data.

#### 2.2.3. 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-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 26 sensor wavelengths	W/m <sup>2</sup> -nm / 0 – 3x10 <sup>7</sup>			
Sflux	real	Solar flux for 26 sensor wavelengths	W/m <sup>2</sup> -nm / 0 – 3x10 <sup>7</sup>			

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

#### 2.2.4. 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
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Control File	1	namelist.nml Runtime parameters (generated by driver script)		ASCII
	2	SOMPS_npp_IDP STime <sup>§</sup> _noaa_ops.h5	IDPS outputs of SDR data	HDF5
IDPS Granula	3	GONPO_npp_IDP STime <sup>§</sup> _noaa_ops.h5	IDPS outputs of GEO data	HDF5
File	4	SOMTC_npp_IDP STime <sup>§</sup> _noaa_ops.h5	IDPS outputs of SDR data for OMPS NM	HDF5
	5	GOTCO_npp_IDP STime <sup>§</sup> _noaa_ops.h5	IDPS outputs of GEO data for OMPS NM	HDF5
	6	band_centers.txt	Wavelengths and assumed bandpass FWHM for each measurement channel	ASCII
	7	cloud_ground_pres sure.nc	Cloud pressure data	netCDF
	8	mrgapprf.dat	Merged a priori ozone climatology	ASCII
Ancillary	9	O3_CLIM13.DAT	A priori ozone profile climatology	ASCII
File	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

<sup>§</sup>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.

#### 2.3. Theoretical Description

#### **2.3.1.** Physical Description

Comprehensively describe the sensor physics and the associated geophysical phenomenology key to the product retrieval. *(Document Object 15)* **Writers:** Algorithm Scientists.

The Version 8 O3 profile algorithm (V8PRO) is the latest in a series of BUV (backscattered ultraviolet) vertical profile O3 algorithms that have been developed for the SBUV and follow on SBUV/2 instruments. This chapter describes the basis for the V8PRO implementation with emphasis on the changes from the Version 6 O3 profile algorithm (V6A) it is replacing. The V6A is described in *Bhartia* et al. [1996] and in the OMPS Nadir Profile ATBD [*Ball, 2002*]. Both the V6A and V8PRO use optimal estimation to generate maximum likelihood retrievals. See *Rodgers*, [1976] and *Rodgers*, [1990] for theoretical analysis of the properties of this class of retrievals, and *Meijer* et al. [2006] for applications to O3 profile estimation. This chapter also makes frequent references to the two previous chapters' descriptions of the physical basis of the measurements and the modeling techniques that are shared by the V8TOZ and the V8PRO.

The Version 8 vertical profile O3 algorithm (V8PRO) is the first new SBUV/2 algorithm since the Version 6 (V6A) in 1990. 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 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 V6A improvements directly. Finally, the V8A is designed for expansion to perform retrievals for hyperspectral instruments, such as OMI, GOME-2 and the OMPS-NP. 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.

The Solar Backscatter Ultraviolet instruments, SBUV on Nimbus 7 and SBUV/2s on NOAA-9, -11, -14, -16 and -17 -18, are nadir-viewing instruments that infer total column O3 and the O3 vertical profile by measuring sunlight scattered from the atmosphere in the ultraviolet spectrum. *Heath* et al. [1975] describes the SBUV flown on Nimbus-7. *Frederick* et al. [1986], and *Hilsenrath* et al. [1995] describe the follow-on SBUV/2 instruments flown on the NOAA series of spacecraft.

The instruments are all of similar design; nadir-viewing double-grating monochromators of the Ebert-Fastie type. The instruments step through 12 wavelengths in sequence over 24 seconds, while viewing the Earth in the fixed nadir direction with an instantaneous field of view (IFOV) on the ground of approximately 180 km by 180 km. To account for the change in the scene-reflectivity due to the motion of the satellite during the course of a scan, a separate co-aligned filter photometer (centered at 343 nm on SBUV; 380 nm on SBUV/2) makes 12 measurements concurrent with the 12 monochromator measurements. Each sequence of measurements ends with an 8 second retrace, producing a complete set of measurements every 32 seconds on the daylight portions of an orbit.

The OMPS-NP and OMPS-NM continue this set of measurements with instruments using two-dimensional CCD arrays to obtain spectral measurements from 250 nm to 380 nm with approximately 0.4 nm sampleing and 1.1-nm full-width half maximum bandpasses. The instruments are described in *Dittman et al.* 2002.

The instruments are flown in polar orbits to obtain global coverage. Since the BUV O3 measurements rely on backscattered solar radiation, data are only taken on the dayside of each orbit. There are about 14 orbits per day with 26° of longitudinal separation at the equator. Unfortunately, the early NOAA polar orbiting satellites are not sunsynchronous. For example, the NOAA-11 equator crossing times drifted from 1:30 pm (measurements at 30° solar zenith angle or so at the equator) at the beginning of 1989 to 5:00 pm by the end of 1995 (measurements at 70° solar zenith angle). As the orbit drifts, the terminator crossing location moves to lower latitudes and coverage decreases. The OMPS instruments are on platforms with well-controlled orbits maintaned close to 1:30 PM Equator crossing times.

Ozone profiles and total column amounts are derived from the ratio of the observed backscattered spectral radiance to the incoming solar spectral irradiance. This ratio is referred to as the backscattered top-of-atmosphere albedo (TOAA) or top-of-atmosphere reflectance. The only difference in the optical components between the radiance and irradiance observations is the instrument diffuser used to make the solar irradiance measurement; the remaining optical components are identical. Therefore, a change in the diffuser reflectivity will result in an apparent trend in O3. This is the key calibration component for the BUV instruments. See *Hilsenrath* et al. [1995] for a longer discussion.

The spectral resolutions for SBUV(/2) and OMPS double monochromators are all approximately 1.1 nm, full-width at half-maximum (FWHM. The wavelength channels used for Nimbus 7 SBUV were at 256, 273, 283, 288, 292, 298, 302, 306, 312, 318, 331, and 340 nm. The wavelengths for NOAA-9 and the other NOAA SBUV/2 instruments were very similar except that the shortest channel was moved from 256 nm to 252 nm in order to avoid emission in the nitric oxide gamma band that contaminated the SBUV Channel 1 measurements. The OMPS hyperspectral measurements are converted to radiance irradiance ratios and these are linearly interpolated to give values at the target wavelength locations. The OMPS NP on S-NPP has been found to have a 0.015 nm amplitude annual variation in its wavelelength scales related to thermal

changes in the optical bench. The OMPS NP measurements are used for the eight shortest channels and the OMPS NM is used for the four longer ones.

Data from the 256 nm and 252 nm channels are not used in the V8PRO reprocessing for any of the instruments, but the algorithm allows for the use of this channel if desired, for example, in operational processing. The atmospheric O3 absorption decreases by several orders of magnitude over the 252 nm to 340 nm wavelength range. The V8PRO uses a variable number of backscattered ultraviolet measurements depending on the solar zenith angle (SZA) of the observations to maintain its sensitivity to O3 changes in the lower stratosphere. For small solar zenith angles (the sun high in the sky), only six wavelengths are used in the retrievals. They are at 273 nm, 283 nm, 288 nm, 292 nm, 298 nm, and 302 nm. As the SZA increases the 306 nm, then 313 nm and finally the 318 nm channels are added to the retrieval.



Figure 2-3: Sample ozone weighting functions for the seven shortest SBUV/2 channels for two solar zenith angle. Wavelength results for each SZA case are short to log going from top to bottom.

Figure 2-3 shows the sensitivity of the profiling channels to unit O<sub>3</sub> changes at different heights. Because the shortest wavelengths are absorbed before penetrating very far, they only sense the O<sub>3</sub> amounts at the top of the atmosphere. When the sun is higher in the sky (lower SZA), the path length decreases and the photons penetrate farther into the atmosphere – compare the top two cuves in Fig. 3-1.

#### 2.3.2. Mathematical Description

**Forward Model** 

The BUV radiances observed in the profiling wavelength channels (250 nm to 310 nm) vary by over four orders of magnitude. Sample Solar, Earth and TOAA measurements are shown in Fig. 3-2. The contributions to the shorter wavelength ( $\lambda$  < 290 nm) channels are dominated by single scattered photons from the middle and upper stratosphere, while the longer wavelength channels (( $\lambda$  > 290 nm) may have significant contributions from multiple scattering and surface and cloud reflectivity (MSR). See Fig. 1-2. for representative contribution functions for these wavelength ranges. Two different radiative transfer forward models are combined to represent the radiances. One uses a simple single scattering calculation while the other uses look up tables created with the TOMRAD forward model described in Section 2.2. The formulation of the single scattering model and the use of both models are described below.



Figure 2-4: A Sample of Solar Irradiance (Top), Earth radiance (Middle), and Earth albedo (Bottom) measured by NOAA-17 SBUV/2.

#### **Single Scattering Forward Model**

The algorithm uses an internal forward model to estimate the single scattering components of the TOA. For an atmosphere containing only Rayleigh scatterers and O<sub>3</sub>, for a wavelength  $\lambda$ , the optical depth in the atmosphere in the nadir direction, as a function of pressure,  $\tau_{\lambda}(p)$ , can be written as  $\tau_{\lambda}(p) = \int \alpha_{\lambda}(t(p'))x(p') + \beta_{\lambda} dp'$  where, x(p') is the derivative of the column O<sub>3</sub> amount above a pressure p' [x(p) = dX(p)/dp where X(p) is the partial column of ozone from the top of the atmosphere down to pressure p],  $\alpha_{\lambda}(t)$ 

is the O<sub>3</sub> absorption coefficient at temperature t, and  $\beta_{\lambda}$  is the Rayleigh scattering coefficient at a wavelength  $\lambda$ .

At wavelengths below 290 nm, little solar radiation penetrates below 30 km, permitting surface, cloud, and aerosol effects to be ignored. Because radiation is scattered from a region of the atmosphere which is optically thin for scattering, multiple scattering effects may also be ignored. For such cases, the backscattered radiance intensity in Eq. (2.1) can be explicitly written to a high degree of accuracy as

$$R_{\lambda} = (1/4\pi) F_{\lambda} \beta_{\lambda} P(\cos\theta_0) \int \exp[-\int s(p') (\alpha_{\lambda}(t(p'))x(p') + \beta_{\lambda}) dp'] dp$$
(3.1)

Where  $\theta_0$  is the solar zenith angle, s is the slant path factor (air mass factor), P is the Rayleigh phase function,  $F_{\lambda}$  is the solar flux, and p is pressure. The outer integral limits are the surface to the top of the atmosphere. The inner integral limits are pressure p to the top of the atmosphere. This expression for  $R_{\lambda}$  is commonly described as the single scattering radiance. The Rayleigh phase function, P(cos $\theta_0$ ), assuming a depolarization factor of 0.035 (Bates, 1984), can be written as

$$P(\cos\theta_0) = 0.7619 \ (1 + 0.937 \cos^2\theta_0). \tag{3.2}$$

The slant path (air mass), s, for the SBUV/2 or OMPS nadir viewing geometry, can be approximated by 1+sec( $\theta_0$ ) at low solar zenith angles (<60°), or by the Chapman (1931) function at moderate solar zenith angles (<80°). For solar zenith angles greater than 80°, s must be treated as a function of p, calculated by ray-tracing. The slant pass must also be modified to account for the increase in neutral atmosphere as a function of pressure increments with increasing height, that is, the gravity gradient. This increases the scatters by a factor of [1+H(p)/R<sub>e</sub>]<sup>2</sup> where R<sub>e</sub> is the radius of the Earth at a surface at 1 atmosphere and H(p) is the physical height the layer at pressure p is above this surface. We will work with the top of atmosphere albedos (TOAA) I=R/F.

The algorithm computes the single scattered albedos and the corresponding Jacobians of partial derivatives with respect to layer O<sub>3</sub> amounts for given BUV channels by using a double discretization of Eq. (3.1) in atmospheric pressure and wavelength bandpass. The discretization in pressures represents the atmosphere by using 81 pressure layers with constant logarithmic spacing. Approximation of the atmosphere by using the pressure layers transforms the integral in Eq. 3.1 into a discrete sum with x(p) transformed into a corresponding discrete set of O<sub>3</sub> layer amounts, and t(p) into a discrete set of mean layer temperature values. The partial derivatives of I with respect to O<sub>3</sub> layer amounts can be efficiently computed by multiplying the component results for I by the appropriate  $-s\alpha$  values and computing the appropriate sums.

The second discretization concerns the representation of the wavelength channels 1.1-nm bandpasses. These are modeled by using a discrete set of 21 wavelengths spaced at 0.1 nm intervals around each bandpass center, multiplying the calculated  $I_{\lambda}$  for each wavelength by the relative bandpass contribution, and summing to provide the estimate of the full channel. Results using finer spacing and additional weighting to model solar variations produced small additional improvements.

#### **Multiple Scattering Forward Model**

The multiple-scattering forward model used in the V8PRO is the same radiative transfer forward model described in Section 2.2, namely, TOMRAD. Again it is used to create look-up tables of radiances and Jacobians. In this case, the look-up tables give the relative changes between the MSR results and the single scattering results. That is, the tables give the ratio of full multiple scattering and reflectivity simulations and partial derivatives to corresponding single scattering ones. This means that they give the values to transform single scattering and reflectivity estimates. Additional tables with the sensitivity of the Jacobian tables to O<sub>3</sub> layer changes allow the algorithm to track changes in the partial derivatives even when the iterations of the O<sub>3</sub> profile solution, described in the next section, move away from the standard profiles used to generate the tables.

#### **Spectroscopic Constants**

The same data sets are used for the O3 cross-sections and Rayleigh scattering as are described in Section 2.2.1.

#### 2.3.3. Retrieval Algorithm

The retrieval algorithm uses a maximum likelihood retrieval combining *a priori* O3 profile information with the BUV measurements. The longer channel measurements are used to provide an initial total O3 estimate (used only to generate the first guess) and a cloud/surface reflectivity estimate (adjusted for photometer variations but fixed for the retrieval). The measurement vector is represented by  $Y_M$  and contains the natural logarithm of the TOAAs for the shorter channels (the number of channels is varied with solar zenith angle and total O3); the unknown O3 profile is represented by a vector X and its components are the values for layer O3 content in Dobson Units for each of 21 pressure layers; and the corresponding 21-layer *a priori* O3 profile is represented by a vector  $X_A$  as defined in the next section. The 21 layers are defined by 21 pressure levels at

That is, with 5 layers per decade of pressure or approximately 3-KM spacing, except for the last layer; it extends to the top of the atmosphere. Some calculations are performed on finer layers with a total of 81 sublayers (20 per decade or pressure) each approximately 0.8-KM thick. The following sections describe the components of the maximum likelihood retrieval, namely: the *a priori* O3 profile data set, the *a priori* and measurement covariance matrices, the forward model linearization and Jacobian construction, and the iteration and its stopping criteria.

#### 2.3.4. Version 8 Algorithm A Priori Profiles

The *a priori* profile database was created from 15 years (1988-2002) of ozonesonde measurements and SAGE (Version 6.1) and/or UARS-MLS (Version 5) data. Over 23,400 sondes from 1988-2002 were used in producing this climatology. The data were "filtered", *i.e.*, obvious bad data points were removed. Balloons that burst below 250 hPa were discarded. Data from bouncing balloons were sorted by pressure. Note: No total O3 correction factor (TOMS or Dobson) filtering was used. The stations were weighted equally for each band so that we do not introduce any longitudinal biases (*e.g.*, Resolute and Nyalesund have equal weights in December even though Nyalesund has three times as many sondes as Resolute for that month). The SAGE data was also "filtered" for bad retrievals. Average profiles from ozonesondes and SAGE are merged over a 4-km range with the sonde weight decreasing from 80 to 60 to 40 to 20% and the SAGE weight increasing correspondingly. The covariance matrices are used in generating the BUV operational and reprocessed retrieval products.

The *a priori* profile data set is the same as the 3-dimensional standard profile data set for the V8TOZ. It gives the climatological O3 profile averages for 18 10° latitude bands and 12 months. The lowest layer from the *a priori* program will differ from that used in the retrieval if the surface pressure is not 1 atmosphere. These profiles are used to determine the discrete *a priori* O3 profile used in a specific retrieval by linear interpolation in latitude and day. This discrete O3 profile is designated by a vector  $X_A$  whose components are layer amounts in Dobson Units. Another data file with terrain heights as a function of latitude and longitude is used to generate the surface pressure for given latitude and longitude, and the lowest layers are truncated as appropriate.

#### 2.3.5 Retrieval Formulation

The retrieval formulation begins with a linearization of the discretized forward model about a first guess for the O<sub>3</sub> profile, X<sub>0</sub>. This first guess is from a total O<sub>3</sub> and latitude interpolation of the 21 standard profiles used in the V8TOZ. In addition to the O<sub>3</sub> profiles, look up tables contain the forward model adjustments to convert single scattering estimate to the full multiple scattering and reflectivity TOAA values. The Y<sub>0</sub> [TOAA forward model estimates of log(R/F)] are found by using the single scattering model applied to X<sub>0</sub> for the current measurements viewing conditions and adjusting them to calculate the full multiple scattering values by using the factors from the look-up table tables (with the same total O<sub>3</sub> and latitude interpolations). The linearization is given by

$$Y = Y_n + K_n (X - X_n) \quad n = 0, 1, ...$$
(3.3)

Where  $Y_n$  is the forward model estimate after iteration n,  $X_n$  is the O<sub>3</sub> profile estimate after iteration n, and  $K_n$  is the Jacobian matrix of partial derivatives of the components of Y with respect to the components of X ( $\partial y_i / \partial x_j$  where individual  $y_i$  and  $x_j$  represent log of TOAA for a BUV channel and an O<sub>3</sub> pressure layer amount, respectively) evaluated at  $X_n$ . The partial derivative coefficients in K are calculated by using the O<sub>3</sub> profile for the previous iteration  $(X_n)$  and constitute the weighting function. They measure the sensitivity of the radiance at a particular wavelength to changes in O<sub>3</sub> in the different layers in the profile.

The iterative solution proceeds by generating the optimal estimation (maximum likelihood) solution for the current linearized problem by using the following calculation

$$X_{n+1} = X_{A} + S_{A}K^{T} \left[ K_{n}S_{A}K_{n}^{T} + S_{M} \right]^{-1} \left[ Y_{M} - Y_{n} \right] - K_{n} \left( X_{A} - X_{n} \right) \right]$$
(3.4)

Where  $X_n$  is the discrete O<sub>3</sub> profile from iteration n,  $X_{n+1}$  is the new discrete O<sub>3</sub> profile estimate,  $X_A$  is the discrete *a priori* O<sub>3</sub> profile as described in Section 3.3.1,  $Y_M$  is the vector of measurements from the SBUV/2 or OMPS NP for the profiling channels;  $Y_n$ and  $K_n$  are the forward model and Jacobian estimates for an atmosphere containing layer O<sub>3</sub> amounts,  $X_n$ ; and  $S_A$  and  $S_M$  are the *a priori* and measurement covariance matrices, respectively. The algorithm uses the size of the RMS change in X from one iteration to the next as a stopping criterion.

The theoretical algorithm does not place any restrictions on the covariance matrices  $S_A$  and  $S_M$  except that they should be non-negative definite with the proper dimensions. In practice, the V8PRO uses an artificial  $S_A$  matrix constructed by specifying the diagonal to give a constant percent variability for the O<sub>3</sub> in each layer and then using a scale height correlation to specify the off diagonal values. The  $S_M$  matrix is taken to be a diagonal matrix as the SBUV/2 and OMPS show little correlation in noise between channels.

For reprocessing, the *a priori* covariance used in the maximum likelihood retrieval is an artificial construct as follows: the diagonal elements correspond to 50% variance and the non-diagonal covariance elements fall off with a correlation length of twelve fine layers (approximately 10 KM). The measurement covariance,  $S_M$  is a multiple of the identity matrix and the diagonal entries correspond to radiance errors of 1% in each channel. For operational processing this is increased to 2%. We are considering assigning more realistic noise levels to these entries as functions of instrument performance in the different channels and at different signal levels.

The computation of the Jacobian matrix, K, is performed in three steps at each iteration. First the internal single scattering model is used to estimate the partial derivatives for the single scattering radiances, second multiple scattering adjustments to the partial from the previous iteration are updated with the table partial sensitivities and the change in the retrieved profile from the last iteration, finally, the multiple scattering partial adjustments are applied in a first order (linear) expansion to generate the new full multiple scattering and reflectivity Jacobian from the one for the previous iteration.

#### 2.3.6. Averaging Kernels

Unlike the V6 profile retrieval algorithm, the V8a has a true separation of the *a priori* and first guess. This simplifies averaging kernel analysis. Averaging kernels are an algebraic construct of the linearized problem given in Eq. (3.4). One can manipulate

the equation to give an expression involving the Averaging Kernel Matrix, A. This produces the solution in terms of an impulse-response formulation. Specifically,

$$X_R = X_A + A (X_T - X_A) = (I-A) X_A + A X_T$$
 (3.5)

where  $X_T$  is the true profile,  $X_A$  is the *a priori* O3 profile, and  $X_R$  is the retrieved O3 profile.

If one considers how the retrieved profile responds to a unit change in a single layer of the true profile, then the impulse response interpretation of the averaging kernel is clear. These retrieval impulses to truth deviations from the *a priori* profile can plotted as profile responses to changes at a specified level.

Figures 3.3a, 3.3b and 3.3c give some sample averaging kernel plots to help to describe the V8PRO retrieval capabilities. They shows Averaging Kernels (AK) (for fractional changes in O3 layer amounts) at 15 middle and upper stratospheric pressure levels. The short horizontal lines on the right side of the graph show the pressure levels and point to the corresponding AK. The horizontal and AK lines' styles correspond. In general, the (fractional) variation in the mixing ratio reported by BUV retreivals at a given pressure level is a weighted average of the (fractional) variation of the real mixing ratio at surrounding altitudes, relative to the *a priori* profile. Since the V8PRO *a priori* profiles have no inter-annual variation, the AKs also show how the algorithm would smooth a long-term trend in O3 mixing ratio. Note, however, that individual BUV profiles usually have structures that are finer than those implied by the AKs; these structures come from the assumed *a priori* profile, rather than from the measurements themselves.



Figure 2-5a: Averaging kernel as fractional layer changes for an equatorial profile and viewing condition.



Figure 2-5b: Averaging kernel as fractional layer changes for a mid-latitude profile and viewing condition.



Figure 2-5c: Averaging kernels as fractional layer changes for a high latitude profile and viewing condition.

Figure 2-5a shows typical AKs at the equator. The AKs show best resolution of ~6 km near 3 hPa, degrading to ~10 km at 1 and 20 hPa. Outside this range the retrieved profiles have little information. For example, the (fractional) variation in O<sub>3</sub> mixing ratio seen at 0.5 hPa actually represents the (fractional) variation from the region around 1 hPa, and the variation around 50 hPa represents the variation from around 30 hPa.

Figure 2-5b shows typical AKs for March at 40N latitude. At this latitude the 50 hPa AK does capture some of the atmospheric variation, albeit with a FWHM resolution of ~11 km. In general, the upper AKs get progressively better as the solar zenith angle increases, and the lower AKs become better as the O<sub>3</sub> density peak drops in altitude. Figure 3.3c shows typical AKs for March at 80N latitude. One can see the improvement in AKs for the upper portions of the profile, especially the 0.5, 0.7, 1, and 1.5 hPa AKs, in capturing the atmospheric variation more accurately than in Figs. 2 and 1, with better resolution of ~6 km at 0.7 hPa.

The AK results presented here use the  $S_A$  and  $S_M$  covariance matrices applied for the reprocessed product retrievals. The operational retrievals use an  $S_M$  matrix with larger entries to allow for the greater uncertainty in the operational calibration. The averaging kernels for the operational implementation are slightly broader than those shown here.

#### 2.3.7 Error Analysis

The V8PRO combines backscattered ultraviolet measurements and *a priori* profile information in a maximum likelihood retrieval placing it in the same class of retrievals as V6A described in *Bhartia* et al. [1996]. The following list gives an overview of how errors will be reduced:

1. The V8PRO has new set of *a priori* profiles varying by month and latitude leading to better estimates in the troposphere (where BUV methods lack retrieval information) and allowing simplified comparisons of SBUV/2 and OMPS results to other measurement systems (in particular, to Umkehr ground-based O<sub>3</sub> profile retrievals which use the same *a priori* data set).

2. The V8PRO has a true separation of the *a priori* and first guess. This simplifies averaging kernel analysis. Examples and further information on the smoothing errors were provided above.

3. The V8PRO has improved multiple scattering and cloud and reflectivity forward model estimates. These corrections are updated as the algorithm iterates toward a solution.

4. Some errors present in the V6A will be reduced or corrected. These include a reduction of errors on the order of 0.5% down to 0.1% by improved fidelity in the bandpass modeling, and a reduction in errors from inelastic scattering by including average adjustments for each channel for these effects.

5. The V8PRO incorporates several *ad hoc* V6A improvements directly. These include better modeling of the effects of the gravity gradient, better representation of atmospheric temperature influences on O<sub>3</sub> absorption, and better corrections for wavelength grating position errors.

6. The V8PRO uses improved terrain height information compared to the V6A and gives profiles relative to a better climatology of surface pressure.

7. The V8PRO is designed to allow the use of more accurate external and climatological data (e.g., snow and ice fields) and to allow simpler adjustments for changes in wavelength selection and calibration.

8. Finally, the V8PRO is designed for expansion to perform retrievals for hyperspectral instruments, such as OMI, GOME-2 and the Nadir Profiler in OMPS so future comparisons will be simplified.

The V8PRO uses the same profiling wavelengths and measurements as those used by the V6A and both algorithms are maximum likelihood retrievals. This means that the retrieval responses to measurement noise and bias will be similar if similar  $S_M$  and  $S_A$  matrices are used. There is a fundamental difference in their use or non-use of total ozone information for the ozone profile retrievals. The V6A uses the total ozone estimate for the scan sequence as a constraint on the maximum likelihood retrieval. The V8PRO has no such constraint so the total profile ozone is controlled by the profile wavelength information and the *a priori* profile amounts. This means that the best total ozone estimates from the V8TOZ may differ from the total of the profile retrievals. The profile total will have less sensitivity to real tropospheric ozone changes, but they will also have less sensitivity to tropospheric aerosol effects which are difficult to model.

#### **Forward Model Errors**

The V8PRO has several refinements in this area. The single and multiple scattering forward model applications for the V8PRO are improved relative to V6, and the *a priori* climatological O<sub>3</sub> data are from a more complete set of profiles with improved information on seasonal and latitudinal variations of tropospheric ozone. The new *a priori* data set leads to improvements in the retrievals in the troposphere where the BUV retrievals lack information and to easier interpretation of the source of information in the retrieved profiles. This means that the radiances attributed to the stratosphere are more accurate.

The internal single scattering forward model has itself been made more accurate as follows: It now uses a discrete sum of monochromatic results to represent the instrument bandpass and incorporates a temperature profile in the O<sub>3</sub> cross-section calculation (instead of using "effective" cross sections without any pressure dependence as was the case for the V6A); and it corrects for the gravity gradient in scatterers with height.

The V6 profile algorithm made an initial adjustment to the radiances to account for MSR differences with the single scattering model and then proceeded with only single scattering calculations as it iterated to a solution. The V8PRO has improved multiple scattering and cloud and reflectivity modeling by the use of the MSR tables of corrections and Jacobians. These are used to update the MSR versus single scatter adjustments after each iteration in the retrieval process. In addition, the average effects of inelastic Raman scattering (RRS) are computed for each profiling wavelength and a set of adjustments are used to represent these contributions to first order. Both forward models use a new data based of terrain height (surface pressure) with improvements in both its accuracy and spatial resolution.

#### **Inverse Model Errors**

The discretization of the atmosphere in 0.8-KM layers and the discretization of the bandpass at 0.1-nm wavelength intervals were chosen to reduce modeling errors from these sources to 0.1% levels. The smoothing error of the retrievals (inherent in any remote-sensing maximum-

likelihood inversion) can be observed in the Averaging Kernel results in the previous section. As noted, resolution varies from 6 KM in the middle/upper stratosphere to 20 KM in the troposphere.

#### Temperature

The current implementations use a set of climatological temperature profiles which capture the main seasonal and latitudinal features of the temperature variations. If improved estimates, *e.g.*, from current forecasts or assimilations are available, then these can used. By noticing that the radiances in Eq. 3.1 depend on the product of the ozone amount at pressure p, x(p) multiplied by the ozone cross section as a function of the temperature at pressure p,  $\alpha(t(p))$ , one can switch between partial derivatives with respect to x to those with respect to t by using the chain rule. Specifically,

 $\partial y_i / \partial t_j = \partial y_i / \partial x_j [x_j / \alpha_j] d\alpha_j / dt_j$  (3.6)

for channel i and layer j.

#### **2.3.8. Instrumental Errors**

This section investigates the response of the profile retrievals to errors in the measurements. It begins by showing results from sensitivity calculations for wavelength-independent and wavelength-dependent errors. A full day of reprocessing retrievals for NOAA-17 SBUV/2 for September 1, 2006 is used as the baseline. These profiles are compared to those from additional runs of the same day with perturbations to the measurements. The sensitivity results are followed by estimates of the size and occurrence of a variety of instrument and measurement errors include calibration uncertainties, stray light and wavelength scales.



Figure 2-6: Difference in retrieval responses for  $\pm 1\%$  uniform measurement errors at all profiling wavelengths at 16 latitudes (every 10° from 75S to 75N)

Figure 2-6 shows the effects of a uniform shift in the calibration of all the profile wavelength measurement channels. The thick solid line gives the paired results for 45N latitude when all channels are increased by 1% or all channels are deceased by 1%. The dotted lines give the paired results for other the full range of latitudes covered by the SBUV/2 or OMPS NP, 80S to 80N. The retrieval algorithm interprets a 1% increase in the radiances at all profiling channels at 45N as a decrease in the middle and upper stratospheric ozone amounts of approximately 2%, little change in the lower stratosphere, and an increase in the tropospheric ozone amounts of 1%.

Figure 2-7 shows the effects of -0.5% shifts in individual channels for six profiling wavelength channels – 273 nm, 283 nm, 288 nm, 292 nm, 298 nm and 302 nm — for a retrieval at 45N latitude. The six curves go from the shortest channel to the longest in the following order; Thick Solid, Thick Dotted, Thick Dashed, Thin Solid, Thin Dotted, Thin Dashed. In general, the larger retrieval differences are found higher in the atmosphere for the shorter wavelengths and lower in the atmosphere for the longer ones. These features will follow the pattern of the contribution function shown in Fig 3-1, moving higher with increases in SZA or ozone amounts. The S<sub>A</sub> and S<sub>M</sub> matrices were in their reprocessing configuration for these sensitivity tests.



Figure 2-7: Difference in retrieval response for -0.5% measurement errors at individual profile wavelengths – 273, 283, 288, 292, 298 and 302-nm channels for the 273-nm to 302-nm channels at 45N latitude.

#### **Radiometric Calibration**

The measurement errors modeled in Figs. 3-4 & 3-5 were chosen because they are representative of the types of uncertainties expected in the TOAA calibration for the SBUV/2 instruments, that is, errors in the overall calibration of all the channels combined with errors in the relative calibration of individual channels. Details on the calibration of the SBUV/2 instruments are beyond the scope of this ATBD. Material on the methods for maintaining this

calibration and estimates of the success of their application can be found in the following articles and their references: *Herman* et al. [1991], *Bhartia* et al. [1995], *Hilsenrath* et al. [1995], *Cebula and DeLand* [1998], *Flynn* et al. [2000], *Huang* et al. [2003], *Deland* et al. [2002], and *Flynn* et al. [2006]. The OMPS instruments have better designs to maintain their calibration. A reference on the results for OMPS from the first two years was provided in the first chapter.

#### **Stray Light**

The BUV measurements are affected by two types of stray light – in band stray light (IBSL) and out-of-band stray light (OBSL). Instruments behaviors range from very small stray light errors for both of these sources (*e.g.*, NOAA-9 SBUV/2) to significant impact from both (*e.g.* NOAA-17 SBUV/2).

Figure 3-6 shows evidence of OBSL for the NOAA-17 SBUV/2 from ground measurements of sun on the diffuser. The symbols show the actual measurements at the discrete SBUV/2 wavelengths. The solid line gives an extrapolation using ozone retrieved from the longer wavelength measurements to predict the true signal for the shorter wavelengths. The atmosphere is a very strong filter below 290 nm, so the true signals should be below the instrument noise level (given by the horizontal line). The measurements for the shortest five wavelengths all show significant OBSL. Empirical methods using correlations between longer channel reflectivity variations and shorter channel stray light have been used to devise models and corrections. After applying these corrections, systematic errors are removed, but some sceneand SZA-dependent errors at the 0.5% level remain.



Figure 2-8: Out-of-Band Stray Light for NOAA-17 SBUV/2 observed in Ground Test.

Figure 3-7 shows evidence of IBSL for NOAA-17 SBUV/2 in the 292-nm channel. The presence of this "bump" is exposed by using a linear extrapolation of the radiances versus SZA for the 70° to 75° range and subtracting it from the data. The 10% radiance error at 292 nm is caused by sunlight scattered from the instrument or spacecraft into the entrance aperture. Fortunately, the phenomenon is limited to high SZAs and predictable satellite azimuth angles. Unfortunately, when it occurs it affects most of the profiling wavelengths, and is seen on the SBUV/2 instruments on NOAA-14, -17 and -18, although only at high SZA and only in one hemisphere for any orbit.



Figure 2-9: Onset of In-band Stray Light at 77° SZA as Seen in NOAA-17

The measurements affected by these two stray light errors are either corrected to the 0.5% or better level (in the case of OBSL) or flagged as bad retrievals (in the case of IBSL). A correction to bring the errors for the IBSL case below the 0.5% level is under development.

The OMPS NP and NM also have stray ligth contributions to the measuremetns. These were well-characterized in the laboratory and have been used to create measurement based correction models. These have been implemented in the Level 1 (SDR) OMPS processing.

#### Wavelength Scale and Bandpass

Measurements at lamp or solar lines can also be used to track the wavelength scale and monitor the bandpass shape. Figure 3-8 shows the results of continuous scan mode measurements (taken every 0.15 nm) across four Hg-Lamp lines. This data is analyzed to estimate the line centers as functions of the monochromator grating positions providing accurate characterization of sensor wavelength scale at the 0.01 nm level. The nearly-triangular, 1.1-nm instrument bandpass is also confirmed. These characterizations reduce the errors from these sources to the 0.1% levels. (Figure 3-8 is reproduced from *DeLand* et al [2002].)



Figure 2-10: Signal Levels across a Hg-Lamp Line from Continuous Scan

The OMPS NP and OMPS NM have wavelength scale variations related to changes in the thermal invironements. The OMPS NM located at the side of the the instrument structure shows intra-orbit variations with an amplitude of 0.02 nm. Because of the hyperspectral nature of the measurements, we are able to estimate these shifts on a spectrum by spectrum basis. Both a direct granule to granule estimate and correction and an offline model of the intra-orbital pattern have been implemented to adjust the OMPS NM wavelength scale as part of the N-value computation. The OMPS NP shows little intra-orbit wavelength scale variation but the solar measurements show an annual cycle. This is not currently corrected and represent an error source for the ozone profile products. We plan to implement a correction in 2015.

#### 2.4. Algorithm Output

Describe the output data products - not format - at a level of detail to determine if the product meets user requirements. *(Document Object 17)* **Writers:** Algorithm Scientists.

Table 2-3 describes the external distributed NDEV8P file and Table 2-2 describes the variables in 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 2-3 NDE Ozone Profile File

#### Table 2-4 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	Aerosol Index	5 x 5	Unitless	-100~ 100

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	Float				
	32 bit		5 x 5	Unitless	
AlgorithmFlag TO3	Intege	Algorithm Flag	_		0~10
	r				
	32 hit		5 x 5	Unitless	
Ascending_Descendi		1=Descending,	5.5	Unitess	0.1
ng	intege	0=Ascending			0~ 1
		A. 10 mars - f	<b>F F</b>	Nh	
AverageSolutionResi		Average of	SXS	invalue	0~ 20
dual	⊢loat	residuals			
	32 hit	Averaging	20 x 20 x 5 x 5	DU/DU	
AveragingKernel	Float	kernel matrix			-500~ 500
	Tioat	at 20 layers			
ChannelBandnase	20 hit	The FWHM	13	Nanomet	
		band width		ers	0.2~ 50
HIVI	Float	assumption			
	32 bit	Cloud	5 x 5	hPa	40 4500
CloudPressure	Float	Pressure			10~ 1500
ColumnAmountO3 P	32 hit	Ozone Profile	5 x 5	Dobson	
rofile	Float	Column Sum	0.00	Units	0~ 10000
ColumnAmountO3 T	32 hit		5 x 5	Doheon	
	52 Dit	Step 3 ozone	3.4.5	Linito	10~ 1000
03		The correlation	4	Uniticac	
CorrelationLength			1	Unitless	0~ 81
	Float	length	<b></b>		-
EffectiveCloudFractio	32 bit	Radiative	5 X 5	Unitless	0~ 100
n	Float	Cloudtraction			
		The apriori	1	Unitless	
	32 hit	error			
ErrorApriori	Float	covariance			0~ 10
	i iuai	matrix			
		assumption			
	32 bit		5 x 5	Unitless	
ErrorCode Profile	Intege	Profile Return			0~19
	r	Code			0 10
	•	Error flag from	5 x 5	Unitless	
	32 bit	the Total	0.00	Ondess	
ErrorCode_TO3	Intege				0 ~ 10
	r	ozone			
		computation	4.5		
	32 bit	Ihe	10	Unitless	
ErrorMeasurement	Float	measurement			0~ 10
		error			
	32 hit	Final	10 x 5 x 5	Unitless	
FINALRESIDUAL		Residuals from			-100~ 100
	Float	solution profile			
	32 bit	Initial	10 x 5 x 5	Unitless	100 100
INTTALKESIDUAL	Float	Residuals from			-100~ 100

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		solution profileprofile			
IndexLongestChannel	32 bit Intege r	Index of longest channel used in retrieval	5 x 5	Unitless	1 ~ 500
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	The pressure levels of the	15	hPa	0.5~ 50.0
_	Fillat	ratio profile			
Reflectivity331	32 bit	Computed reflectivity at	5 x 5	Unitless	
	Float	the 331nm			0~ 100
		Computed	5 x 5	Unitless	
Reflectivity340	32 bit Float	reflectivity at the 340nm channel			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

		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
	Float	year			

#### 2.5. Performance Estimates

#### 2.5.1. Test Data Description

Description of data sets used for V&V, including unit tests and system test, either explicitly or by reference to the developer's test plans, if available. This will be updated during operations to describe test data for maintenance. *(Document Object 31)* **Writers:** Development Testers

#### 2.5.2. Sensor Effects

Characterize sensor effects that may contribute to retrieval error. Include the following effects if relevant:

o Flowed-through effects of sensor noise (radiometric, thermal, or other) on the quality of products, using text and graphics (scatter plots, image displays, etc.). o Flowed-through effects of calibration errors (radiometric, including structured

scenes and response versus scan, or any sensor biases) on the quality of products, using text and graphics.

o Flowed-through spatial and spectral error effects (pointing and geolocation errors, apodization, modulation transfer function (MTF), point-spread function (PSF), out-ofband (OOB) response, near-field stray light, Earth shine, solar contamination, polarization, cross talk, etc.) on the quality of products, using text and graphics.

o Flowed-through effects of un-modeled or neglected geophysical phenomena on the quality of products, using text and graphics.

(Document Object 18) Writers: Algorithm Scientists.

#### 2.5.3. Retrieval Errors

Accuracy of products, as measured by V&V testing, and compared to accuracy requirements. Refer to relevant test reports. *(Document Object 39)* Writers: Algorithm Scientists and Development Testers should collaborate

Organize the various error estimates into an error budget, presented as a table. Error budget limitations should be explained. Describe prospects for overcoming error budget limitations with future maturation of the algorithm, test data, and error analysis methodology. (Document Object 19) Writers: Algorithm Scientists.

To be defined.

#### 2.5.3.1. Practical Considerations

#### 2.5.4. Numerical Computation Considerations

Describe how the algorithm is numerically implemented, including possible issues with computationally intensive operations (e.g., large matrix inversions, truncation and rounding). (Document Object 21) Writers: Development Programmers.

#### 2.5.5. Programming and Procedural Considerations

Describe any important programming and procedural aspects related to implementing the numerical model into operating code. *(Document Object 22)* **Writers:** Development Programmers.

#### 2.5.6. Quality Assessment and Diagnostics

Describe how the quality of the output products and the retrieval itself is assessed, documented, and any anomalies diagnosed. *(Document Object 23)* **Writers:** Algorithm Scientists.

#### 2.5.7. Exception Handling

List the complete set of expected exceptions, and describes how they are identified, trapped, and handled. *(Document Object 24)* **Writers:** Development Programmers.

The algorithm check for non-physical values for radiances

#### 2.6. Validation

Describe how the algorithm has been or should be validated at a level of detail appropriate for the current algorithm maturity. *(Document Object 26)* **Writers:** Algorithm Scientists.

#### 3. ASSUMPTIONS AND LIMITATIONS

#### 3.1. Performance Assumptions

Describe all assumptions that have been made concerning the algorithm performance estimates. Note any limitations that apply to the algorithms (e.g., conditions where retrievals cannot be made or where performance may be significantly degraded. To the extent possible, the potential for degraded performance should be explored, along with mitigating strategies. *(Document Object 20)* **Writers:** Algorithm Scientists.

#### 3.2. Potential Improvements

Describe potential future enhancements to the algorithm, the limitations they will mitigate, and provide all possible and useful related information and links. *(Document Object 25)* **Writers:** Algorithm Scientists.

#### 4. REFERENCES

List all references to external documents.

- Ball Aerospace & Technology Corporation, <u>Algorithm Theoretical Basis Document (ATBD)</u> <u>Nadir Profile Ozone) for the Ozone Mapping and Profiler Suite (OMPS) of the National</u> <u>Polar-Orbiting Operational Environmental Satellite System (NPOESS) Program,</u> Document Number – IN0092A-108 CI Number – SS0052Am January 2002.
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Web References

The Solar Backscatter Ultraviolet instrument (SBUV/2) measurements fly on the NOAA

Polar-orbiting Operation Environmental Satellites (POES). Information on these sensors and products is available in sections 3.8, 7.4 and 9.7 of the NOAA-KLM User's Guide at

http://www.ncdc.noaa.gov/docs/klm/.

- Activation and evaluation reports and other calibration documents can be found at http://www.orbit.nesdis.noaa.gov/smcd/spb/calibration/icvs/sbuvdoc.html
- Calibration and validation monitoring can be found in the ultraviolet instrument links at http://www.orbit2.nesdis.noaa.gov/smcd/spb/calibration/icvs/index.html
- Additional monitoring information and the V8 Fortran code are available from links at <u>http://www.orbit.nesdis.noaa.gov/smcd/spb/ozone/</u>

ftp://www.orbit.nesdis.noaa.gov/pub/smcd/spb/ozone/code

Additional documentation and product validation are contained on theV8PRO data DVD available at

http://disc.sci.gsfc.nasa.gov/data/datapool/TOMS/DVD-ROMs/

The following documents with information on the V8TOZ and V8PRO implementation in the operational processing at NOAA are available from NOAA/NESDIS:

- Solar Backscattered Ultraviolet Radiometer (SBUV/2) Operational Ozone Product System Version 8, System Maintenance Manual, Dec. 2006, Prepared by Q. Zhao & J. Selekof.
- Solar Backscattered Ultraviolet Radiometer (SBUV/2) Operational Ozone Product System Version 8, System Description Document, Dec. 2006, Prepared by Q. Zhao & J. Selekof.
- Solar Backscattered Ultraviolet Radiometer (SBUV/2) Operational Ozone Product System Version 8, Interface Control Document, Dec. 2006, Prepared by Q. Zhao & J.

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