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Joint Polar Satellite System (JPSS) Operational Algorithm Description (OAD) Document for Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Intermediate Product (IP) Software

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Goddard Space Flight Center
Greenbelt, Maryland

National Aeronautics and
Space Administration

Joint Polar Satellite System (JPSS) Operational Algorithm Description (OAD) Document for Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Intermediate Product (IP) Software

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Preface

This document is under JPSS Ground Algorithm ERB configuration control. Once this document is approved, JPSS approved changes are handled in accordance with Class I and Class II change control requirements as described in the JPSS Configuration Management Procedures, and changes to this document shall be made by complete revision.

Any questions should be addressed to:

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Change History Log

Revision	Effective Date	Description of Changes (Reference the CCR & CCB/ERB Approve Date)
Original	06/03/2011	This version incorporates **474-CCR-11-0085** which converts Operational Algorithm Description (OAD) Document for OMPS Nadir Profile (NP) Intermediate Product (IP), Rev B, dated 08/18/2010 to a JPSS document, Rev -. This was approved by the JPSS Ground Algorithm ERB on June 3, 2011.
Revision A	01/18/2012	**474-CCR-11-0271:** This version baselines 474-00067, Joint Polar Satellite System (JPSS) Operational Algorithm Description (OAD) Document for Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Intermediate Product (IP) Software, for the Mx6 IDPS release. This CCR was approved by the JPSS Algorithm ERB on January 18, 2012.
Revision B	05/14/2013	**474-CCR-13-0948:** This version authorizes 474-00067, JPSS OAD Document for OMPS NP IP Software, for the Mx 7.0 IDPS release. Includes Raytheon PCR032720; CCR-474-13-0916/ECR-ALG-0037: Update applicable OAD filenames/template/Rev/etc. for Mx7 Release.
Revision C	11/06/2013	**474-CCR-13-1288:** This version authorizes 474-00067, JPSS OAD Document for OMPS NP IP Software, for the Mx 8.0 IDPS release. Includes administrative changes authorized by interoffice memo and Raytheon PCR034526; Update OAD to account for new OMPS NP IP data names, in Tables 5 and pages 22 and 23.
Revision D	09/03/2015	**474-CCR-15-2591:** This version authorizes 474-00067, JPSS OAD Document for OMPS NP IP Software, for the Mx 8.11 IDPS release. Includes Raytheon PCR050751, Child: PRO: OAD: 474-CCR-15-2502: Improved Algorithm for OMPS Nadir Profiler - V8Pro, affects entire document.

NATIONAL POLAR-ORBITING OPERATIONAL ENVIRONMENTAL SATELLITE SYSTEM (NPOESS)

OPERATIONAL ALGORITHM DESCRIPTION DOCUMENT FOR OMPS NADIR PROFILE (NP) INTERMEDIATE PRODUCT (IP)

SDRL 141
SYSTEM SPECIFICATION SS22-0096

RAYTHEON COMPANY
INTELLIGENCE AND INFORMATION SYSTEMS (IIS)
NPOESS PROGRAM
OMAHA, NEBRASKA

IAW DFAR 252.227-7036, Raytheon hereby declares that, to the best of its knowledge and belief, the technical data delivered under Subcontract No. 7600002744 is complete, accurate, and complies with all requirements of the Subcontract.

TITLE: NATIONAL POLAR-ORBITING OPERATIONAL ENVIRONMENTAL SATELLITE SYSTEM (NPOESS) OPERATIONAL ALGORITHM DESCRIPTION DOCUMENT FOR OMPS NADAR PROFILE (NP) INTERMEDIATE PRODUCT (IP)

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Engineering & Manufacturing Development (EMD) Phase
Acquisitions &Operations Contract

CAGE NO. 11982

Operational Algorithm Description For OMPS NP IP

Document Date: Nov 07, 2011

Document Number: D38045
Revision: C4

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This document has been identified per the NPOESS Common Data Format Control Book – External Volume 5 Metadata, D34862-05, Appendix B as a document to be provided to the NOAA Comprehensive Large Array-data Stewardship System (CLASS) via the delivery of NPOESS Document Release Packages to CLASS

Northrop Grumman Space & Mission Systems Corp. **Space Technology** One Space Park Redondo Beach, CA 90278	NORTHROP GRUMMAN Raytheon

Revision/Change Record

Document Number D38045

Revision	Document Date	Revision/Change Description	Pages Affected
---	2-27-04	Initial Release	All
---	10-21-04	Reflects Science To Operational Code Conversion	All
---	05-04-05	Reflects NGST comment corrections plus inserted new logo and updated upper right header date, title/signature page dates, Revision/Change Record	All
---	7-11-05	Removed export markings per 26May05 official policy change and under section 1.3.3, Source Code and Test Data References, inserted a more detailed table listing paths to find applicable source code within the ClearCase configuration management tool	All
---	7-13-05	Per a Dan Antzoulatos 11Jul05 comment, reworded the table under Section 1.3.3 defining a path on ClearCase to find applicable source code.	Pg 2
A	6-11-09	Converted to document format specified in D41851 (IDPS converted Rev --- into the new format and delivered to NG for inclusion in drop 5.2 as Rev A to distinguish it from previous OAD revisions. Rev B is the culmination of the Science-to-operations conversion, associated tech memos, and the TIM-ARB-ACCB process. Rev B will be the first ACCB approval of this OAD.)	All
B1	12-01-09	Updated subcontract number and Table 1. Updated RFA Nos. 422 & 308.	Title pgs, 1-2
B2	1-21-10	Updated with changes from TM 2009.510.0059	All
B2	3-23-10	Updated OAD to reflect the build Maintenance A operational algorithm.	All
B3	3-30-10	Incorporated CCPR comments and prepared for SDRL delivery.	All
B4	4-22-10	Incorporated additional CCPR comments to resolve difference with the TC and other OADs.	All
B	8-18-10	Incorporated SDRL comments (none) and prepared for TIM/ARB/ACCB	All
C1	10-20-10	Updated due to document convergence	All
C2	11-18-10	Updated due to PCR023770	Table 2
C3	11-05-11	Updated due to PCR027205	Table 5
C4	11-07-11	Updated due to PCR026083	Tables 5, 8 & 9

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INTRODUCTION

1.1 Objective

The purpose of the Operational Algorithm Description (OAD) document is to express, in computer-science terms, the remote sensing algorithms that produce the National Polar-Orbiting Operational Environmental Satellite System (NPOESS) end-user data products. These products are individually known as Raw Data Records (RDRs), Temperature Data Records (TDRs), Sensor Data Records (SDRs) and Environmental Data Records (EDRs). In addition, any Intermediate Products (IPs) produced in the process are also described in the OAD.

The science basis of an algorithm is described in a corresponding Algorithm Theoretical Basis Document (ATBD). The OAD provides a software description of that science as implemented in the operational ground system -- the Data Processing Element (DPE).

The purpose of an OAD is two-fold:

1. Provide initial implementation design guidance to the operational software developer.
2. Capture the “as-built” operational implementation of the algorithm reflecting any changes needed to meet operational performance/design requirements.

An individual OAD document describes one or more algorithms used in the production of one or more data products. There is a general, but not strict, one-to-one correspondence between OAD and ATBD documents.

1.2 Scope

The scope of this document is limited to the description of the core operational algorithms required to create the Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Version 6 Intermediate Product (IP) (V6Pro) and the Version 8 IP (V8Pro). The theoretical bases for these algorithms are described in the OMPS Nadir Profile Ozone Algorithm Theoretical Basis Document (ATBD), 474-00026 with the V8 ATBD material.

1.3 References

1.3.1 Document References

Table 1. Reference Documents

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Table 1. Reference Documents

Document Title	Document Number/Revision	Revision Date
OMPS Nadir Profile Ozone Algorithm Theoretical basis Document (ATBD)	474-00026	Latest
NPOESS Calibration and Validation Plan Vol. 5: OMPS	D34484	17 Dec 2002
OMPS Algorithm Test and Verification Plan	D38041	13 Feb 2004
OMPS Algorithm Verification Status Report	D36812 Version 1.0	31 Mar 2003
Operational Algorithm Description Document for Ozone	474-00081	Latest

Document Title	Document Number/Revision	Revision Date
Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Sensor Data Record (SDR)		
Operational Algorithm Description Document for Ozone Mapping and Profiler Suite (OMPS) Total Column (TC) Sensor Data Records (SDR)	474-00077	Latest
JPSS CGS Data Processor Inter-subsystem Interface Control Document (DPIS ICD) Vol I – IV	IC60917-IDP-002	Latest
JPSS Environmental Data Record (EDRIP) Production Report for NPP	474-00012	Latest
JPSS Environmental Data Record (EDR) Interdependency Report (IR) for NPP	474-00007	Latest
JPSS Common Data Format Control Book - External - Block 1.2.4 (All Volumes)	474-00001-01-B0124 CDFCB-X Vol I 474-00001-02-B0124 CDFCB-X Vol II 474-00001-03-B0124 CDFCB-X Vol III 474-00001-04-01-B0124 CDFCB-X Vol IV Part 1 474-00001-04-02-B0124 CDFCB-X Vol IV Part 2 474-00001-04-03-B0124 CDFCB-X Vol IV Part 3 474-00001-04-04-B0124 CDFCB-X Vol IV Part 4 474-00001-05-B0124 CDFCB-X Vol V 474-00001-06-B0124 CDFCB-X Vol VI 474-00001-08-B0124 CDFCB-X Vol VIII	Latest
NPP Command and Telemetry (C&T) Handbook	D568423 Rev. C	30 Sep 2008
IDPS Processing SI Common IO Design Document	DD60822-IDP-011 Rev. A	Latest
Joint Polar Satellite System (JPSS) Program Lexicon	470-00041	Latest
NPP Mission Data Format Control Book and App A (MDFCB)	429-05-02-42-02_MDFCB	Latest
NGAS Tech Memo - Updates to the NP IP OAD Corresponding to Delivery 5.2	TM 2009.510.0059	28 Oct 2009

1.3.2 Source Code References

Table 2. Source Code References

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Table 2. Source Code References

Reference Title	Reference Tag/Revision	Revision Date
OMPS Science Algorithms Delivery	ISTN_OMPS_NP_NGST_3.2	22 Jan 2005
OMPS NP IP Operational software	Build 1.3.0.14 (OAD Rev ---)	28 Jun 2005
OMPS Science Algorithms Delivery	ISTN_OMPS_NP_IP_NGST_5.2 (OAD: TM 2009.510.0059)	30 Nov 2009
OMPS NP IP Operational software	Build Maintenance A 2 (MaintA-2) (OAD Rev B2)	23 Mar 2010

Reference Title	Reference Tag/Revision	Revision Date
SDRL	(OAD Rev B3)	30 Mar 2010
ACCB (no code updates)	OAD Rev B	18 Aug 2010
Convergence Update (No code update)	(OAD Rev C1)	20 Oct 2010
PCR023770 metadata only	Maintenance Build 1.5.5.A (OAD Rev C2)	18 Nov 2010
PCR027205 (x-ref PCR026006)	(OAD Rev C3)	05 Nov 2011
PCR026083	(OAD Rev C4)	07 Nov 2011
OAD transitioned to JPSS Program – this table is no longer updated.		

2.0 ALGORITHM OVERVIEW

This document is the operational algorithm description for the NP ozone IP/EDR of the OMPS algorithms. The OMPS NP ozone algorithms are adopted from the heritage National Oceanic and Atmospheric Administration (NOAA) Solar Backscatter Ultraviolet Spectrometer (SBUV) Version 6 operational Product Processor algorithm (V6Pro) and the Version 8 operational Product Processor algorithm (V8Pro).

The OMPS NP SDR algorithm's output format is based on the OMPS Total Column SDR algorithm's output format. Reference the OMPS NP SDR OAD, 474-00081, and TC SDR OAD, 474-00077, for more information. To link the SDR output to the processor, a module called sdr2pmf was created to convert radiances and other data from the OMPS NP SDR to one of the input types (known as the SBUV/2 Product Master File (PMF) format) that can be ingested. The processing relationship is nominally illustrated in cartoon format in Figure 1.

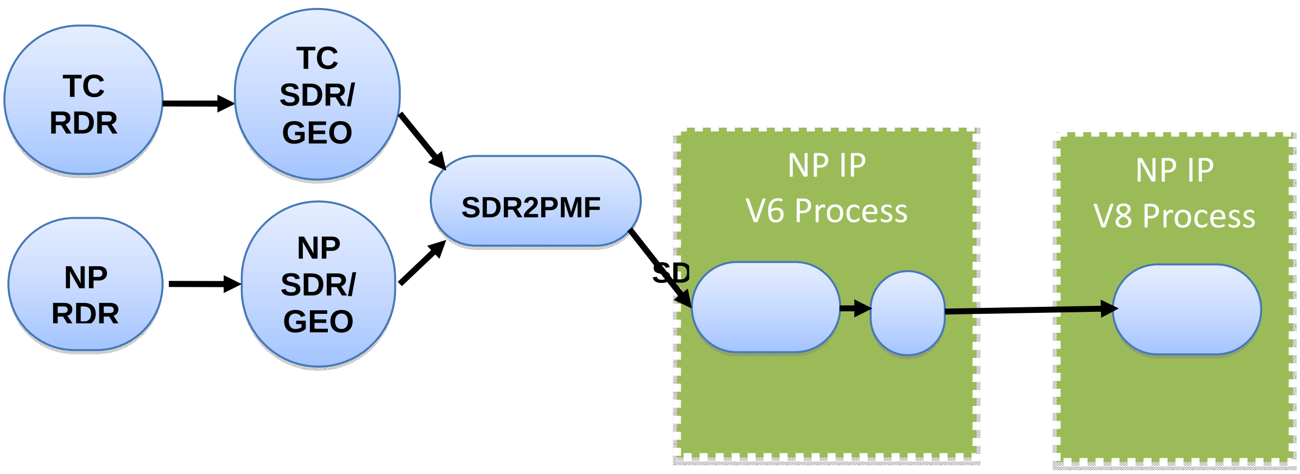

Figure 1. Nominal Processing Chain Associated with the OMPS NP Ozone Algorithm

The module **sdr2pmf** converts data from the NP SDR, NP SDR GEO, TC SDR, TC SDR GEO, and the TC granulation of ancillary surface pressure into PMF format. The sdr2pmf executable is integrated into the front end of the IP/EDR algorithm. Currently the input to the science algorithm is in legacy PMF format. To find appropriately collocated data from the TC chain, data for the same granule and usually the +1 granule must be obtained. With a 37.44s granule, there is an 80% chance that one or more swath of TC data is needed from the +1 granule.

The program **pprod_62.f** is the main driver for the SBUV/2 product processor.

2.1 OMPS Nadir Profile Version 6 IP Description

2.1.1 Interfaces

The NP IP algorithm is initiated by the Infrastructure (INF) Software Item (SI) to begin processing the data. The INF SI provides tasking information to the algorithm indicating which granule is processed. The Data Management System (DMS) SI provides data storage and retrieval capability. The interface to these SIs is implemented by a library of C++ classes. The interfaces to these other SIs are shown in Figure 2.

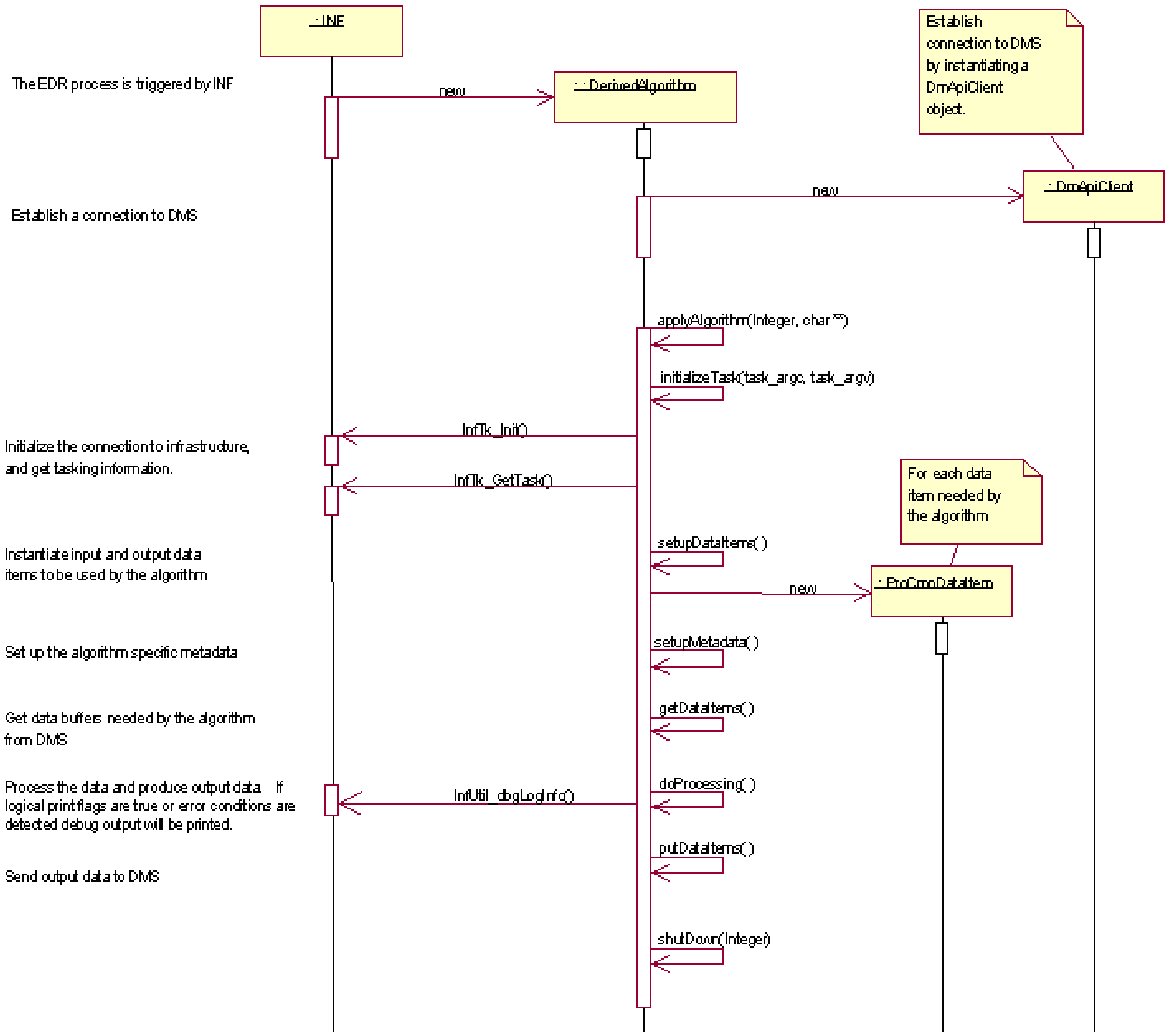

Figure 2. IPO Model Interface to INF and DMS

2.1.1.1 Inputs

The NP IP science processing requires two inputs: an auxiliary Look-Up Table (LUT) and a PMF record that contains NP SDR information. The PMF data record is described in Table 3. Since the SBUV/2 system takes radiance measurements for 12 wavelengths over a time span of 32 seconds, three considerations are made to be included in the PMF: Information on the beginning; information on viewing conditions at start of the time span; and average viewing conditions for the time scan. Since OMPS takes measurements for all wavelengths simultaneously, only one set of viewing conditions is needed, and the information contained in the input PMF may therefore look redundant. Also, for SBUV/2 the PMF contains values corresponding to the photometer. For OMPS these values are replaced with measurements corresponding to radiances taken by the nadir TC sensor at 380 nm. Not all data needed to produce the NP IP is contained in the PMF file. The algorithm also ingests the NP SDR directly to pass quality flags: sun glint, SAA, and eclipse. Refer to the CDFBC-X, 474-00001, for a detailed description of the inputs.

Table 3. Nadir Profile PMF Intermediate Input

Input	Word	Type	Description	Original Source	Units
REC	1	Integer*4	Data record number	Input SDR file	Unitless
SEQ	2	Real*4	Logical sequence number	Input SDR file	Unitless
ORBIT	3	Real*4	Orbit number	Input SDR file	Unitless
YEARDAY (V8Pro use)	4	Real*4	Day of year + 1000*year	Input SDR file	Days
SEC	5	Real*4	UT seconds at start of integration period	Input SDR file	Seconds
LATBEG	6	Real*4	Latitude (for SBUV/2 was latitude at beginning of scan)	Input SDR file	Degrees
LONBEG	7	Real*4	Longitude (for SBUV/2 was longitude at beginning of scan)	Input SDR file	Degrees
LATTOZ (V8Pro use)	8	Real*4	Latitude (for SBUV/2 was average latitude for total ozone wavelengths)	Input SDR file	Degrees
LONTOZ (V8Pro use)	9	Real*4	Longitude (for SBUV/2 was average longitude for total ozone wavelengths)	Input SDR file	Degrees
SZATOZ (V8Pro use)	10	Real*4	Solar Zenith Angle (for SBUV/2 was average solar zenith angle for total ozone wavelengths)	Input SDR file	Degrees
NPHOTTOZ (V8Pro use)	11-14	Real*4	Total column sensor N value for 380 nm channel (for SBUV/2 was the photometer N values for the profile wavelengths)	Input SDR file	N value
NMONOTOZ (V8Pro use)	15-18	Real*4	Total column sensor N values for the 340, 331, 318, and 312 nm channels	Input SDR file	N value
TOZGAIN	19	Real*4	Unused for OMPS	-	-
GPOS	20	Real*4	Unused for OMPS	-	-
SPARE	21-26	Real*4	Unused for OMPS	-	-
APRTOZ	27	Real*4	A pair total ozone	Output from SBUV/2 retrieval algorithm	Dobson Unit (DU)
APRSENS	28	Real*4	A pair sensitivity	Output from SBUV/2 retrieval algorithm	(N value / DU)
APRREF	29	Real*4	A pair average reflectivity	Output from SBUV/2 retrieval algorithm	Percent
APRWT	30	Real*4	A pair weight (weighting factor in TOZ calc)	Output from SBUV/2 retrieval algorithm	Unitless
BPRTOZ	31	Real*4	B pair total ozone	Output from SBUV/2 retrieval algorithm	DU
BPRSENS	32	Real*4	B pair sensitivity	Output from SBUV/2 retrieval algorithm	(N value / DU)
BPRREF	33	Real*4	B pair average reflectivity	Output from SBUV/2 retrieval algorithm	Percent
BPRWT	34	Real*4	B pair weight (weighting factor in TOZ calc)	Output from SBUV/2 retrieval algorithm	Unitless
BSTTOZ	35	Real*4	Best total ozone	Output from SBUV/2 retrieval algorithm	DU
CPRTOZ	36	Real*4	C pair total ozone	Output from SBUV/2 retrieval algorithm	DU
PRESS	37	Real*4	Pressure of reflecting surface	Output from SBUV/2 retrieval algorithm	Atm

Input	Word	Type	Description	Original Source	Units
BSTREF	38	Real*4	Best reflectivity	Output from SBUV/2 retrieval algorithm	Percent
CPRSENS	39	Real*4	C pair sensitivity	Output from SBUV/2 retrieval algorithm	(N value / DU)
TOZCOD	40	Real*4	Total ozone error code	Output from SBUV/2 retrieval algorithm	Unitless
TABLEINDX	41	Real*4	Table selection scheme index	Output from SBUV/2 retrieval algorithm	Unitless
ICE	42	Real*4	Snow/ice code	Output from SBUV/2 retrieval algorithm	Unitless
PHOT_MON_R_DIFF	43	Real*4	Photometer-monochromator reflectivity difference (not used for OMPS NP)	Output from SBUV/2 retrieval algorithm	Percent
TERRPRESS	44	Real*4	Terrain pressure	Input SDR file	Atm
DPRTOZ	45	Real*4	D pair total ozone	Output from SBUV/2 retrieval algorithm	DU
SO2INDEX	46	Real*4	SOI (sulfur dioxide index)	Output from SBUV/2 retrieval algorithm	Unitless
B2PRTOZ	47	Real*4	B prime pair ozone	Output from SBUV/2 retrieval algorithm	DU
LATPRO	48	Real*4	Latitude (for SBUV/2 was average latitude for profile)	Output from SBUV/2 retrieval algorithm	Degrees
LONPRO	49	Real*4	Longitude (for SBUV/2 was average longitude for profile)	Output from SBUV/2 retrieval algorithm	Degrees
SZAPRO	50	Real*4	Solar zenith angle (for SBUV/2 was average solar zenith angle for profile)	Output from SBUV/2 retrieval algorithm	Degrees
NPHOTPRO	51-58	Real*4	N values interpolated from the radiances from the 145 wavelengths of the NP sensor to the SBUV/2 wavelengths (for SBUV/2 were the photometer N values)	Input SDR file	N value
NMONPRO	59-66	Real*4	N values interpolated from the radiances from the 145 wavelengths of the NP sensor to the SBUV/2 profiling wavelengths (for SBUV/2 were the N values of the profiling wavelengths)	Input SDR file	N value
GAIN	67-68	Real*4	Unused for OMPS	-	-
FRSTGUESS	69-80	Real*4	First guess profile for layers	Output from SBUV/2 retrieval algorithm	DU
FRSTGUESSTOZ	81	Real*4	Total ozone for first guess	Output from SBUV/2 retrieval algorithm	DU
QCORR	82-91	Real*4	Q values corrected for multiple scattering and reflectivity contributions	Output from SBUV/2 retrieval algorithm	Unitless
INITRES	92-101	Real*4	Initial residues	Output from SBUV/2 retrieval algorithm	Percent
MSCATCORR	102-106	Real*4	Corrections to Q for longer channels	Output from SBUV/2 retrieval algorithm	Unitless

Input	Word	Type	Description	Original Source	Units
REFWAVE	107-111	Real*4	Reflectivities for longer channels	Output from SBUV/2 retrieval algorithm	Percent
MSCATSENS	112-116	Real*4	Sensitivity of correction to total ozone	Output from SBUV/2 retrieval algorithm	Unitless
MSCATMIX	117-121	Real*4	Multiple scattering mixing fraction	Output from SBUV/2 retrieval algorithm	Unitless
FINLRES	122-131	Real*4	Final residues	Output from SBUV/2 retrieval algorithm	Percent
LYRPRO	132-143	Real*4	Final profile in 12 layers top to bottom	Output from SBUV/2 retrieval algorithm	DU
LYRSTD	144-155	Real*4	Standard deviation of final profile	Output from SBUV/2 retrieval algorithm	Percent
TOZPRO	156	Real*4	Total ozone for solution profile	Output from SBUV/2 retrieval algorithm	DU
PROCOD	157	Real*4	Ozone profile error code	Output from SBUV/2 retrieval algorithm	Unitless
C	158	Real*4	C parameter for c-sigma calculation	Output from SBUV/2 retrieval algorithm	Unitless
SIGMA	159	Real*4	Sigma parameter for c-sigma calculation	Output from SBUV/2 retrieval algorithm	Unitless
MIXPRO[1]	160-178	Real*4	Volume mixing ratio at 19 pressure levels from spline of profile	Output from SBUV/2 retrieval algorithm	ppmv
FRSTGSSTD	179-190	Real*4	Standard deviation of first guess profile	Output from SBUV/2 retrieval algorithm	Percent
QSTDEV	191-200	Real*4	Standard deviation of corrected values	Output from SBUV/2 retrieval algorithm	Unitless
ITER	201	Real*4	Number of iterations of retrieval algorithm	Output from SBUV/2 retrieval algorithm	Unitless
VOLCANO	202	Real*4	VCI (volcano contamination index)	Output from SBUV/2 retrieval algorithm	Unitless
SPARE	203	Real*4	Unused for OMPS	-	-
DPRESENS	204	Real*4	D pair sensitivity	Output from SBUV/2 retrieval algorithm	(N value / DU)
BSPRESENS	205	Real*4	B prime pair sensitivity	Output from SBUV/2 retrieval algorithm	(N value / DU)
ZABEG	206	Real*4	Solar zenith angle (for SBUV/2 was solar zenith angle at beginning of scan)	Input SDR file	Radians x 10^4
ZAEND	207	Real*4	Solar zenith angle (for SBUV/2 was solar zenith angle at end of scan)	Input SDR file	Radians x 10^4

[1] Mass mixing ratios (μgm/gm) are divided by 1.657 to obtain ozone volume mixing ratios (ppmv).

2.1.1.1.1 Look-Up Tables

Table 4.

Nadir Profile IP LUT

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Table 4. Nadir Profile IP LUT

Parameter	Word(s)	Dimension	Description	Units
Spectral information data record				
Record ID	1	real	Record ID	Unitless
WLEN	2-13	real(12)	Bandcentered Wavelengths	Nm
CCR wavelength	14	real	Not used by OMPS	-
ALFA0	15-26	real(12)	Effective absorption coefficients	$(atm\text{-}cm)^{-1}$
CCR ALFA0	27	real	Not used by OMPS	-
BETA	28-39	real(12)	Rayleigh scattering coefficients	atm^{-1}
CCR BETA	40	real	Not used by OMPS	-
Spare	41-180	real(140)	Spares (not used by OMPS)	-
Multiple scattering coefficients data record (for use with NP wavelengths to determine profile)				
Record ID	1	real	Record ID	Unitless
QLOG	2-2301	real(10,23,5,2)	Values of log Q (10 sza's, 23 profiles, 5 wavelengths, and 2 pressures)	Unitless*
QSLOG	2302-4601	real(10,23,5,2)	Values of single-scattered log Q (10 sza's, 23 profiles, 5 wavelengths, and 2 pressures)	Unitless*
FRAC	4602-6901	real(10,23,5,2)	Values of reflected fraction	Unitless*
SBT	6902-7131	real(23,5,2)	Value of atmospheric surface backscatter fraction	Unitless
Total ozone tables data record (for use with TC wavelengths used to determine total column ozone)				
Record ID	1	real	Record ID	Unitless
XLOGIO	2-2761	real(10,23,6,2)	Values of log I0	Unitless*
TBYI0	2762-5521	real(10,23,6,2)	Values of reflected fractions	Unitless*
SB	5522-5799	real(23,6,2)	Values of atmospheric surface backscatter fractions	Unitless
A priori information data record				
Record ID	1	real	Record ID	Unitless
PROFN	2-254	real(11,23)	Values of *A priori* profile coefficients (11 atmospheric layers x 23 profiles), northern hemisphere	DU
PROFS	255-507	real(11,23)	Values of *A priori* profile coefficients (11 atmospheric layers x 23 profiles), southern hemisphere**	DU
COV	508-652	real(12,12)	Values of *a priori* covariance matrix	Unitless

*Unitless because values normalized using solar flux

**Southern hemisphere is set equal to northern hemisphere

2.1.1.2 Outputs

Table 5. Nadir Profile IP Output

Table 6. Nadir Profile Averaging Kernel IP

. Refer to the CDFBC-X, 474-00001, for a detailed description of the outputs.

Table 5. Nadir Profile IP Output

Output	CDFCB-X Name	Type	Description	Units/Valid Range
	Scan-Level Data Items			
SAA	SAA	UInt8 * 1	South Atlantic Anomaly intensity	Unitless / 0 - 9
	Pixel-Level Data Items			
tcSensorLong	NormalizedRadiance_380nm	Float32 * 1 * 1	TC N value collocated to NP	N Value / Minfloat - Maxfloat
tcSensorShort	NormalizedRadiance_340nm_331nm_318nm_312nm	Float32 * 1 * 1 * 4	TC non-380nm N values collocated to NP	N Value / Minfloat - Maxfloat
Wavelengths	Wavelengths	Float32 * 1 * 1 * 13	Wavelengths used in N Value interpolation	nm /
aPairOzone	A-PairTotalO3	Float32 * 1 * 1	A pair total ozone	DU / 0 - 650
aPairSensitivity	A-PairSensitivity	Float32 * 1 * 1	A pair sensitivity	(N Value / DU) / Minfloat – Maxfloat
aPairReflectivity	A-PairReflectivity	Float32 * 1 *1	A pair average reflectivity	Percent / 0 - 100
aPairWeight	A-PairWeight	Float32 * 1 * 1	A pair weight (weighting factor in TOZ calc)	Unitless / Minfloat - Maxfloat
bPairOzone	B-PairTotalO3	Float32 * 1 * 1	B pair total ozone	DU / 0 - 650
bPairSensitivity	B-PairSensitivity	Float32 * 1 * 1	B pair sensitivity	(N Value / DU) / Minfloat – Maxfloat
bPairReflectivity	B-PairReflectivity	Float32 * 1 *1	B pair average reflectivity	Percent / 0 - 100
bPairWeight	B-PairWeight	Float32 * 1 * 1	B pair weight (weighting factor in TOZ calc)	Unitless / Minfloat - Maxfloat
bestOzone	ColumnAmountO3	Float32 * 1 * 1	Best total ozone	DU / 0 - 650
cPairOzone	C-PairTotalO3	Float32 * 1 * 1	C pair total ozone	DU / 0 - 650
reflSurfPressure	reflSurfPressure	Float32 * 1 * 1	Pressure of reflecting surface	Atm / minfloat - maxfloat
bestReflectivity	BestReflectivity	Float32 * 1 * 1	Best reflectivity	Percent / 0 - 100
cPairSensitivity	C-PairSensitivity	Float32 * 1 * 1	C pair sensitivity	(N Value / DU) / Minfloat - Maxfloat
ozoneErrorCode	Ozone Error Flag for Best Ozone	Float32 * 1 * 1	See Table 8. Total Ozone Error Code Descriptions	Unitless / 0.0 – 20.0
tableIndex	tableIndex	Float32 * 1 * 1	Table selection scheme index	Unitless / Minfloat – Maxfloat
iceCode	SnowIceCode	Float32 * 1 * 1	Snow/Ice code	Unitless / Minfloat – Maxfloat
terrainPressure	TerrainPressure	Float32 * 1 * 1	Terrain pressure	Atm / Minfloat - Maxfloat
dPairOzone	D-PairTotalO3	Float32 * 1 * 1	D pair total ozone	DU / 0 – 650

Output	CDFCB-X Name	Type	Description	Units/Valid Range
SOI	SO2index	Float32 * 1 * 1	SOI (sulfer dioxide index)	Unitless / Minfloat – Maxfloat
bPrimeOzone	BPrime-PairTotalO3	Float32 * 1 * 1	B prime pair ozone	DU / 0 – 650
nValProfile	N_Values_InterpolatedToSBUVmon	Float32 * 1 * 1 * 8	N values interpolated from the radiances from the wavelengths produced by the NP sensor to the SBUV/2 profiling wavelengths (for SBUV/2 were the profiling wavelengths)	N value / Minfloat – Maxfloat
firstGuessProfile	FirstGuessO3Profile	Float32 * 1 * 1 * 12	First guess profile for layers	DU / 0 – 650
firstGuessOzone	FirstGuessTotalO3	Float32 * 1 * 1	Total ozone for first guess	DU / 0 – 650
qValCorrect	QValues	Float32 * 1 * 1 * 10	Q values corrected for multiple scattering and reflectivity contributions	Unitless / Minfloat – Maxfloat
initialResidues	InitialResiduals	Float32 * 1 * 1 * 10	Initial residues	Percent / 0 – 100
qCorrLong	QValuesCorrectionsLonger	Float32 * 1 * 1 * 5	Corrections to Q for longer channels	Unitless / Minfloat – Maxfloat
reflectLong	ReflectivitiesLonger	Float32 * 1 * 1 * 5	Reflectivities for longer channels	Percent / 0 – 100
multiScatSens	MultipleScatteringSensitivity	Float32 * 1 * 1 * 5	Sensitivity of correction to total ozone	Unitless / Minfloat – Maxfloat
multiScatMix	MultipleScatteringMix	Float32 * 1 * 1 * 5	Multiple scattering mixing fraction	Unitless / Minfloat – Maxfloat
finalResidue	FinalQValueResidues	Float32 * 1 * 1 * 10	Final residues	Percent / 0 – 100
finalProfile	FinalO3Profile	Float32 * 1 * 1 * 12	Final profile in 12 layers top to bottom	DU / 0 – 650
stdDevProfile	FinalO3Profile_Std	Float32 * 1 * 1 * 12	Standard deviation of final profile	Percent / 0 – 100
ozoneProfile	TotalO3SolutionProfile	Float32 * 1 * 1	Total ozone for solution profile	DU / 0 – 650
ozProfError	Ozone Error Flag for Profile	Float32 * 1 * 1	Ozone profile error code See Table 9	Unitless / Minfloat – Maxfloat
cParameter	CParameter	Float32 * 1 * 1	C parameter for c-sigma calculation	Unitless / Minfloat – Maxfloat
sigmaParameter	SigmaParameter	Float32 * 1 * 1	Sigma parameter for c-sigma calculation	Unitless / Minfloat – Maxfloat
mixingRatio	O3MixingRatio	Float32 * 1 * 1 * 19	Volume mixing ratio at 19 pressure levels from spline of profile	Ppmv / Minfloat - maxfloat
stdDevFirstGuess	FirstGuessO3_Std	Float32 * 1 * 1 * 12	Standard deviation of first guess profile	Percent / 0 – 100
stdDevCorrVals	QValues_Std	Float32 * 1 * 10	Standard deviation of corrected values	Unitless / Minfloat – Maxfloat
numIterations	Iterations	Float32 * 1 * 1	Number of iterations of retrieval algorithm	Unitless / 1 – 5
VCI	VolcanoContaminationIdx	Float32 * 1 * 1	Volcano contamination index	Unitless / Minfloat – Maxfloat

Output	CDFCB-X Name	Type	Description	Units/Valid Range
dPairSensitivity	D-PairSensitivity	Float32 * 1 * 1	D pair sensitivity	(N Value / DU) / Minfloat - Maxfloat
bPrimeSensitivity	BPrime-PairSensitivity	Float32 * 1 * 1	B prime pair sensitivity	(N Value / DU) / Minfloat – Maxfloat
sunGlint	SunGlint	UInt8 * 1 * 1	Sun glint indication (scattering angle and surface type thresholds)	Boolean / 0 - 1
solarEclipse	SolarEclipse	UInt8 * 1 * 1	All or part of the IFOV is affected by a solar eclipse, umbra or penumbra viewing.	Boolean / 0 - 1

Table 6. Nadir Profile Averaging Kernel IP

Output	Type	Description	Units/Valid Range
Pixel-Level Data Items			
Data	Float32 * 1 * 12 * 12	Averaging kernel matrix for retrieval on final iteration	Unitless / Minfloat - Maxfloat

2.1.1.3 I/O Timeliness Requirements

The NP algorithm cannot be executed until TC SDR and NP SDR are available. The NP IP can be produced once all required inputs are available. See Figure 1. Nominal Processing Chain Associated with the OMPS NP Ozone Algorithm

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2.1.2 Algorithm Processing

This class is the derived algorithm for the NP algorithm and is a subclass of the ProCmnAlgorithm class. The class creates a list of input data items that are read from DMS and passes all of the required data into the algorithm itself. When the algorithm has finished processing the data, the output data item is written to DMS.

The purpose of the NP algorithm is to invert nadir radiances to NP ozone and to write the NP output data. The primary data product is layer ozone amounts in 12 layers for all solar zenith angle viewing conditions less than or equal to 80 degrees.

The NP IP source code was written in FORTRAN 77 and then converted to FORTRAN 90 with the interface to IDPS written in C++.

The following sections describe the main driver, subroutines, and the process of how the NP ozone is produced from the OMPS NP sensor measurements. The assumptions contained in the algorithm, data checks, and assessments that are performed in the algorithm are also discussed.

Ozone profiles are derived from the measured albedos using Rodgers optimum statistical inversion technique. Initial information, *a priori* is required since there is not enough information to invert the ozone profile from the measured albedos. The retrieved profile is thus constructed from both the *a priori* information and the measured albedos. The *a priori* information is sometimes referred to as “virtual measurements” because it is an integral part of the profile construction.

The *a priori* information used in the inversion includes a “first guess” profile derived from the best available ozone climatology for the lower portion of the profile and from the three shortest wavelength channel radiances for the uppermost portion. The albedos that such an ozone profile would yield are calculated. The differences between the albedos calculated from the first guess profile and the measured albedos are then used to provide a new set of profile values that are more nearly consistent with both the measured albedos and the first guess profile.

Application of the optimum statistical technique requires not only the measurements and *a priori* profiles but also an assessment of their uncertainty or variance. In the case of the albedo, the uncertainty is characterized by the errors of measurement. The method also requires the covariance of the errors of measurement, to determine how dependent the errors at one wavelength are on the errors at another. For the *a priori* information, the variances and covariances are obtained in the development of the climatology.

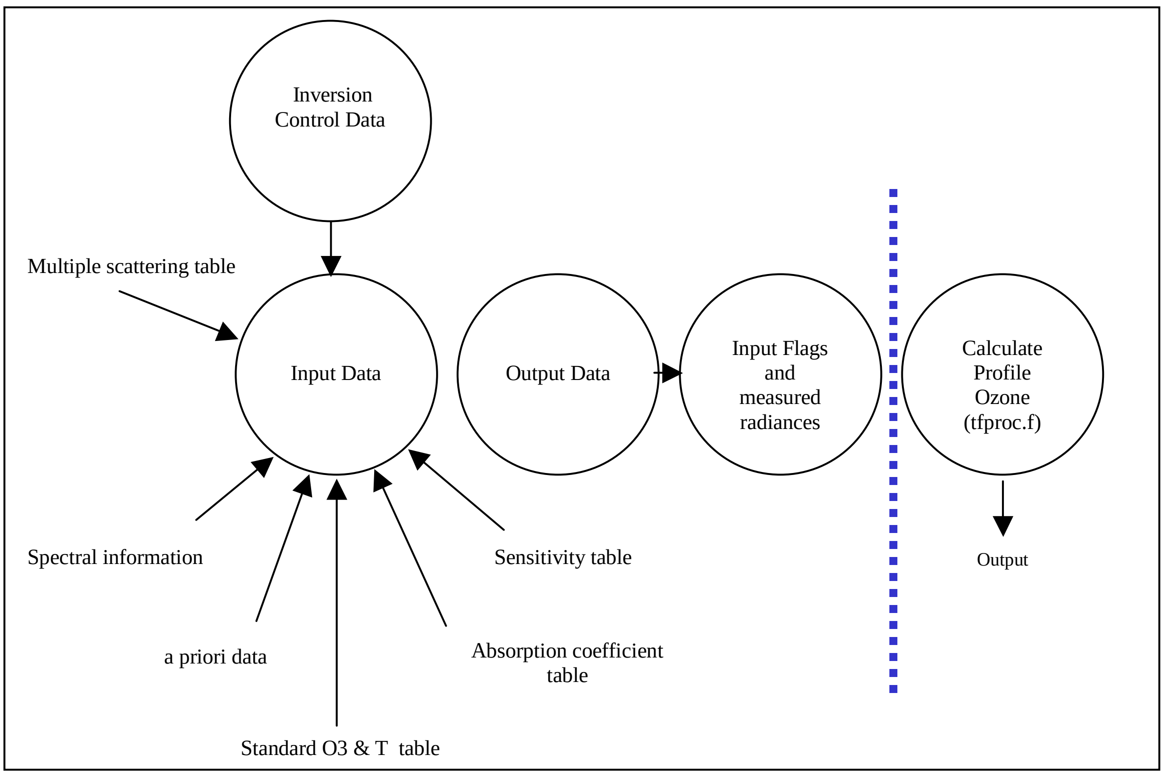

Figure 3. Flow Diagram for the Top-Level Driver pprod_62.f

2.1.2.1 Main Module - pprod_62.f

The main program **pprod (flow described in Figure 4)** is executed once per granule and performs the following preliminary tasks:

1)Retrieves total ozone based on a table lookup and interpolation process. The table has been constructed such that backscattered radiance is a function of total ozone, solar zenith angle, surface pressure, surface reflectivity and latitude.

2) Retrieves profile ozone from the eight shortest wavelength channels using an optimum statistical method and using *a priori* information that includes a first guess profile, an estimate of its variance, the estimated errors in the measurements, and the correlations between profile variance and measurement errors at different levels. The *a priori*

information provides a constraint on which of the solutions consistent with the measurements is accepted and the optimum method governs the way in which the constraint is applied.

See Figure 4 for subroutines 2.1.2.2 to 2.1.2.4.4.

2.1.2.2 Subroutine associateptrs (associateptrs.f)

Subroutine associateptrs maps the DMS pointers to the FORTRAN pointers.

2.1.2.3 Subroutine rednam (rednam.f)

Subroutine **rednam (rednam_63.f)** provides for the ability to print out debug information if logical print flags are configured as true. This subroutine calls **anclv6** when finished.

2.1.2.3.1 Subroutine anclv6 (anclv6.f)

Subroutine **anclv6** initializes various processing parameters.

2.1.2.4 Subroutine tfproc (tfproc.f)

Subroutine **tfproc** is the sub-driver that controls the data processing. It contains a loop that is executed once for each pixel. It calls the total and profile subroutines.

2.1.2.4.1 Subroutine rdatar (rdatar.f)

Subroutine **rdatar** calls **pmfcnv** and sets error codes if input data is detected as bad or out of range.

2.1.2.4.1.1 Subroutine pmfcnv (pmfcnv.f)

Subroutine **pmfcnv** validates input data and sets processing flag to false if errors are detected in data.

2.1.2.4.2 Subroutine total (total_63.f)

Subroutine **total** (**total_63.f**) is the sub-driver that calls the routines for computing total ozone. The measured albedos are expressed in terms of N-values, which are proportional to the logarithm of the albedo. A ratio of albedos then becomes a difference of N-values. Three pairs are defined:

A-Pair = N313 - N331

B-Pair = N318 - N331

C-Pair = N331 - N340

For each of the above N-value differences or pairs, four estimates of total ozone values are calculated. Values of total ozone above 1 atm are derived for reflecting surfaces at 1.0 atm and 0.4 atm. For each of these pressures, ozone values are derived from the two standard latitudes surrounding the actual latitude of the measurements. In each case, N-values for the solar zenith angle of the measurement and the given latitude and pressure level are computed from the table values of I_0, I_s and f_2. These N-values produce table-derived pair N-value differences for total ozone values at 50 matm-cm intervals. Ozone between the terrain height and actual pressure level is subtracted using the amount of ozone between 0.4 and 1.0 atm in the standard profile as a basis, assuming that cumulative ozone is linear with log pressure at these levels. Interpolation of the measured N-value pair difference in the table-derived N-value pairs produces total ozone values for each latitude and pressure. The total ozone values for the two pressures are combined using $P_{Effective} = (1\text{-}w)P_{cloud} + wP_{terrain}$, where w is based on the measured surface reflectivity. The ozone value for the latitude of the measurements is derived by linear interpolation in latitude between the values for the two bordering standard latitudes. Between 15° and the equator, only the profile set for l5° is used; poleward of 75°, only the 75 °profile set is used. An average reflectivity is calculated in the same manner.

2.1.2.4.2.1 Subroutine scanin (scanin.f)

Subroutine **scanin** initializes the total ozone processing for the current scan. The procedure in the subroutine occurs in the following manner:

Compute average latitude, longitude and solar zenith angle as well as the solar zenith angle for each channel.

If $\theta > 88°$, skip this measurement.

Set latitude flag and initial ozone estimate for this sample:

|lat| <= 45°ILAT = 1OZONIN = 260

45°< |lat| <= 75°ILAT = 2OZONIN = 340

|lat| > 75°ILAT = 3OZONIN = 360

Compute the Lagrange interpolation coefficients and the terrain pressure.

Find the starting solar zenith angle table indices.

2.1.2.4.2.2 Subroutine reflec (reflec.f)

Subroutine **reflec** computes an effective surface reflectivity for a defined wavelength and surface pressure. The reflectivity is computed as:

$R = (I - I_0) / [\, I_S f_1 + (I - I_0) f_2 \,]$ as defined in the NP ATBD, 474-00026, equation (59).

2.1.2.4.2.3 Subroutine ozone (ozone.f)

Subroutine **ozone** computes total ozone for a given wavelength pair, surface pressure and reflectivity.

2.1.2.4.2.4 Subroutine prflec (prflec_62.f)

Subroutine **prflec** computes an effective surface pressure base on the reflectivity estimated in subroutine reflec. It estimates a climatological cloud height and then mixes it with the terrain pressure based on reflectivity.

$P_{Effective} = (1-w)P_{cloud} + wP_{terrain}$,

The weighting function w is based on the measured reflectivity. A higher reflectivity generally implies greater cloudiness. Normally, when snow or ice is not present, w is set to unity for R<0.2, to zero for R>0.6, and is obtained by linear interpolation as a function of R for intermediate reflectivities.

2.1.2.4.2.5 Subroutine bestoz (bestoz.f)

Subroutine **bestoz** computes a best ozone estimate by forming weighted combination of total ozone from the A, B and C pair values. The weighting is defined by the sensitivity of each pair.

2.1.2.4.2.6 Subroutine wtsens (wtsens.f)

Subroutine **wtsens** computes pair sensitivities evaluated at input total ozone value. Recomputes pair sensitivities based on total ozone estimate and surface pressure. Table indices are determined from ozone and latitude to compute bracketing N-values. Sensitivities are computed for each wavelength pair, then latitude and pressure mixed if necessary.

2.1.2.4.3 Subroutine profil (profil.f)

Subroutine **profil** is the sub-driver that calculates the Q-values and calls the routines for computing profile ozone.

2.1.2.4.3.1 Subroutine intpro (intpro.f)

Subroutine **intpro** calculates Q-values for the observed radiances of the profile wavelength channels:

$$Q_\lambda = \{4\pi / [\beta_\lambda P (\cos \theta_0)]\} (I_\lambda / F_\lambda)$$

2.1.2.4.3.2 Subroutine slantp (slantp.f)

Subroutine **slantp** calculates the slant path for the profile wavelengths. The slant path (air mass) is approximated by $1 + \sec(\theta_0)$ at solar zenith angles less than 60º and by the Chapman function for $60^\circ \le \theta_0 \le 80^\circ$.

2.1.2.4.3.3 Subroutine chpmn (chpmn.f)

Subroutine **chpmn** computes the chapman function for a given solar zenith angle for a spherical atmosphere containing ozone.

2.1.2.4.3.4 Subroutine frstgs (frstgs.f)

Subroutine **frstgs** calculates the multiple scattering corrections, computes the *a priori* profile and begins computation of the measurement covariance matrix. This subroutine uses total ozone and the long wavelength radiances to calculate the multiple scattering corrections. It also uses latitude, day of year and *a priori* coefficients to obtain the *a priori* profile. It begins the evaluation of the measurement, total ozone and ozone absorption coefficients in constructing the covariance matrix.

2.1.2.4.3.5 Subroutine mscatr (mscatr_63.f)

Subroutine **mscatr (mscatr_63.f)** uses total ozone and long wavelength radiances to obtain multiple scattering correction.

2.1.2.4.3.6 Subroutine sreflc (sreflc.f)

Subroutine **sreflc** computes reflectivity from the measured radiance for a given sun position, ozone, and pressure.

2.1.2.4.3.7 Subroutine aitken (aitken.f)

Subroutine **aitken** performs a cubic spline interpolation.

2.1.2.4.3.8 Subroutine qtabs (qtabs.f)

Subroutine **qtabs** computes the total Q value; its multiple scattered and reflected components, and partial derivative of multiple scattering/reflection component with respect to total ozone, for a given set of input parameters.

2.1.2.4.3.9 Subroutine aprof (aprof.f)

Subroutine **aprof** computes new first guess profile using upper level Thomas-Holland and lower level standard profile.

2.1.2.4.3.10Subroutine tomhol (tomhol.f)

Subroutine **tomhol** uses the Thomas-Holland routine to determine ozone profile by finding the pressure and cumulative ozone corresponding to an optical depth of minimum sensitivity to variations in ozone scale height for each of a set of wavelengths.

2.1.2.4.3.11Subroutine linfit (linfit.f)

Subroutine **linfit** performs a least squares fit to data with a straight line Y = A + B*X.

2.1.2.4.3.12Subroutine alogam (alogam.f)

Subroutine **alogam** evaluates the natural logarithm of the gamma function for argument X greater than zero.

2.1.2.4.3.13Subroutine digama (digama.f)

Subroutine **digama** evaluates the digamma (PSI) function for argument X greater than zero, defined by:

digamma(x) = d(ln(GAMMA(X)))/dX where GAMMA(X) is the gamma function

2.1.2.4.3.14Subroutine stnprf (stnprf.f)

Subroutine **stnprf** retrieves standard profile based on a priori info.

2.1.2.4.3.15Subroutine terp (terp.f)

Subroutine **terp** interpolates between profile ozone amounts based upon latitude.

2.1.2.4.3.16 Subroutine fitpro (fitpro.f)

Subroutine fitpro fits together an upper level Thomas-Holland cumulative ozone profile and a lower level version 6 standard profile into a 12 SBUV layer profile.

2.1.2.4.3.17 Subroutine cubspl (cubspl.f)

Subroutine **cubspl** is a library call that uses cubic spline interpolation.

2.1.2.4.3.18 Subroutine cubsplint (cubsplint.f)

Subroutine **cubsplint** is a library call that uses cubic spline evaluation.

2.1.2.4.3.19 Subroutine splstd (splstd.f)

Subroutine **splstd** obtains mass mixing ratios at 16 standard pressures by interpolation.

2.1.2.4.3.20 Subroutine splset (splset.f)

Subroutine **splset** obtains the coefficients required for cubic spline interpolation.

2.1.2.4.3.21 Subroutine meserr (meserr.f)

Subroutine **meserr** begins evaluation of measurement covariance matrix from errors in measurement, total ozone, and ozone absorption coefficients.

2.1.2.4.3.22 Subroutine pdopt (pdopt.f)

Subroutine **pdopt** calculates the solution profile and its covariance matrix. Pdopt computes iterative solutions of the optimum method until the solution ozone in each of the 12 layers changes by less than 2.5%. In a single iteration the current solution profile is subdivided into 92 layers for calculation of q-values. Differences between these q-values and the measured q-values are used to modify the solution.

2.1.2.4.3.23 Subroutine layrit (layrit.f)

Subroutine **layrit** performs interpolations of ozone amounts from 12-layer scheme to 92 layer scheme for use in profile inversion.

2.1.2.4.3.24 Subroutine frdint (frdint.f)

Subroutine **frdint** uses Newton’s formula for forward interpolation, to the third difference.

2.1.2.4.3.25 Subroutine splnef (splnef.f)

Subroutine **splnef** uses cubic spline interpolation.

2.1.2.4.3.26 Subroutine bkdint (bkdint.f)

Subroutine **bkdint** uses Newton’s formula for backward interpolation, to the third difference.

2.1.2.4.3.27 Subroutine planqd (planqd.f)

Subroutine **planqd.f** uses single scattered Q values and elements of weighting function matrix under plane parallel atmosphere assumption.

2.1.2.4.3.28 Subroutine shelqd (shelqd.f)

Subroutine **shelqd** uses single scattered Q values and elements of weighting function matrix under spherical atmosphere assumption.

2.1.2.4.3.29 Subroutine frstit (frstit_63.f)

Subroutine **frstit (frstit_63.f)** computes initial delq for first iteration of profile retrieval and place solution results in bufpmf.

2.1.2.4.3.30 Subroutine lastit (lastit_63.f)

Subroutine **lastit (lastit_63.f)** computes final residues of profile inversion after last iteration and place results in bufpmf.

2.1.2.4.3.31 Subroutine normeq (normeq.f)

Subroutine **normeq** evaluates and solves normal equations to yield solution profile and its covariance matrix. The subroutine also outputs the profile averaging kernel.

2.1.2.4.3.32 Subroutine invert (invert.f)

Subroutine **invert** inverts real symmetric matrix.

2.1.2.4.3.33 Subroutine vocano (vocano.f)

Subroutine **vocano** computes a SO_2 index and flags conditions that indicate contamination from volcanic eruptions.

2.1.2.4.4 Subroutine wdatar (wdatar.f)

Subroutine **wdatar** updates fields in the output data record.

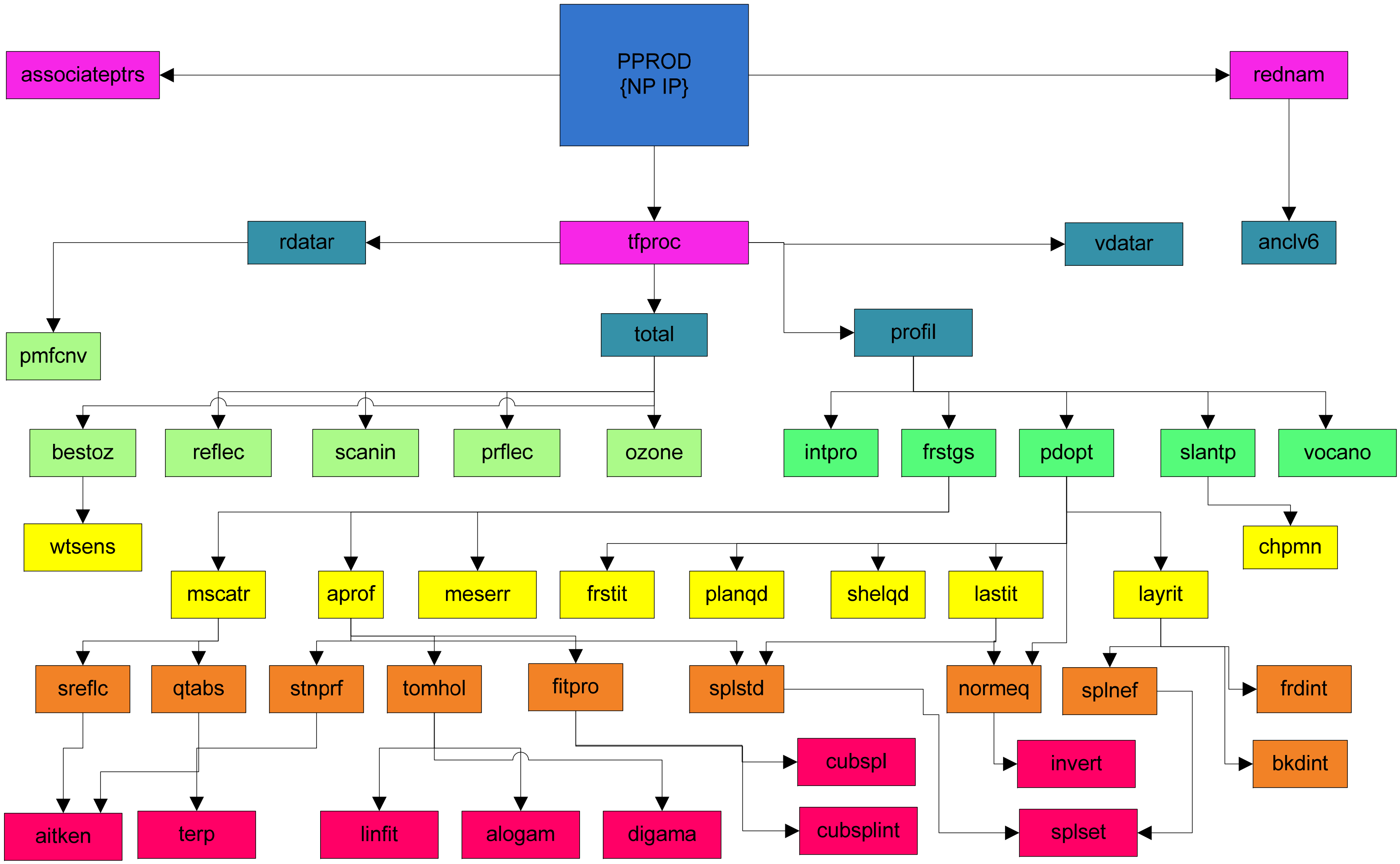

Figure 4. Nadir Profile Flow Diagram

2.1.3 Graceful Degradation

2.1.3.1 Graceful Degradation Inputs

Graceful Degradation details can be found in section 4.3.8 in the EDR Interdependency Report.

Terrain pressure is the only NP IP algorithm input with graceful degradation. This input needs to be granulated to the OMPS NP pixel space and can come from NCEP or a backup climatology database. The NP IP algorithm looks for granulated NCEP and climatology as alternate.

2.1.3.2 Graceful Degradation Processing

None

2.1.3.3 Graceful Degradation Outputs

None

2.1.4 Exception Handling

2.1.4.1 Total ozone flag

The algorithm performs several validity checks for maintaining data quality. Before measured radiances are accepted for use in ozone determination, the solar zenith angle, satellite attitude, and instrument status are checked to ensure the suitability of the radiances and other geophysical input to the algorithm.

The computed best ozone for each pair must be within the range of the radiance tables. For 15° and lower latitudes, the range is 150 to 350 DU, between 15° and 45°, the range is 150 DU to 600 DU, and above 45° the range is 150 DU to 650 DU. If the derived best ozone is outside the range of the tables, it is set to –999 and the quality flag is set to 9.

Next, checks are made on the reflectivity. The reflectivity must be no less than –0.05 and no greater the 1.05. If the reflectivity is outside this range, the best ozone is set to –999 and the quality flag is set to 8.

The best ozone is then compared with the total ozone returned by the profile algorithm. If the two ozone values differ by more than 3 standard deviations, usually about 1.5 percent of the value, the quality flag is set to 5 and best ozone is set to –999. The profile is still derived in this case.

If the data pass flags 9, 8, 7 and 5, the ozone path is calculated:

Ozone path = Best ozone X (1 + sec (solar zenith angle)) / 1000.

Table 7. Ozone Path Quality Flag

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Table 7. Ozone Path Quality Flag

Ozone Path	Quality Flag	Pair used in flag 4 consistency check
1.5	0	A
1.5 – 3.5	1	B
3.5	2	C

If data were taken on the descending (north to south) part of the orbit, the value 10 is added to the flag value.

Table 8. Total Ozone Error Code Descriptions

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Table 8. Total Ozone Error Code Descriptions

Total Ozone Error Code	Description
0.0	Low path (air mass x total ozone < 1.5 atm-cm (ascending)
1.0	High path (1.5 atm-cm ~ air mass x total ozone < 3.5 atm-cm (ascending)
2.0	Very high path (air mass x total ozone > 3.5 atm-cm (ascending)
3.0	Spare (ascending)
4.0	Large disagreement among A,B,C pair total ozone (ascending)
5.0	Best total ozone and profile total ozone inconsistent (ascending)
6.0	Spare (ascending)
7.0	Reflectivity differ by more than 0.05 between consecutive wavelengths (ascending)
8.0	Reflectivity outside –0.05 to 1.05 range (ascending)
9.0	Derived total ozone outside range of tables (ascending)
10.0	Low path (air mass x total ozone < 1.5 atm-cm (descending)
11.0	High path (1.5 atm-cm ~ air mass x total ozone < 3.5 atm-cm (descending)
12.0	Very high path (air mass x total ozone > 3.5 atm-cm (descending)
13.0	Spare (descending)
14.0	Large disagreement among A,B,C pair total ozone (descending)
15.0	Best total ozone and profile total ozone inconsistent (descending)
16.0	Spare (descending)
17.0	Reflectivity differ by more than 0.05 between consecutive wavelengths (descending)
18.0	Reflectivity outside –0.05 to 1.05 range (descending)
19.0	Derived total ozone outside range of tables (descending)
20.0	Inputs to the algorithm were detected to be invalid or out of range

2.1.4.2 Profile ozone flag

If measurements are missing at any wavelength used in the profile calculations, a profile flag of 9 is assigned. If a best ozone value has not been computed in the total ozone algorithm, then a profile error code of 8 is assigned. Next, the reflectivity for the six longest wavelengths, those that are multiply scattered, is checked. If the reflectivity for any of these wavelengths is outside the range –0.05 to 1.05 then a profile error code of 7 is assigned.

The algorithm used the 274 nm and 283 nm Q values to calculate values for C, the cumulative ozone above 1 mbar, and σ, the ratio of the atmospheric scale height to the ozone scale height, assuming that the cumulative ozone x is a function of the pressure p:

$$x = C\, p^{1/\sigma}$$

If σ is outside the range from 0.3 to 0.8, a profile error code of 6 is assigned. If C is greater than 3.0 DU or less than 0.5 DU, profile error code of 5 is assigned.

The observed Q values are compared with the initial Q values calculated from the *a priori* profile, and residues are calculated. A residue is defined by the following equation:

$$r = 100(Q_{obs} - Q_{calc}) / Q_{calc}$$

where Q_{obs} are the Q values derived from the observed radiances and Q_{calc} are the Q values derived from an assumed profile, in this case, the first guess. If this initial residue is larger than 60 percent, a profile error code of 4 is assigned. If the scan passes all checks described thus far, the ozone profile is computed and additional checks are made.

A final residue derived, using the computed profile to derive Q_{calc}, and compared with the standard deviation (σ) of the observed measurements, obtained as the square root of the diagonal term of the measurement error covariance matrix. If the final residue is larger than 3σ, and error code of 3 is assigned. If total ozone returned by the profile algorithm differs by more than 3σ from the total ozone for profiling, an error code of 2 is assigned. If the ozone derived for the three lowest altitude layers differs by more than 5σ from the climatology-derived initial estimate for those layers, an error code of 1, signifying lower-level anomaly, is assigned. A profile that passes all these tests is considered a good profile and is assigned a flag of 0. A value of 10 is added for a descending orbit (north to south).

Table 9. Profile Error Code and Descriptions

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Table 9. Profile Error Code and Descriptions

Profile Error Code	Description
0.0	Good profile (ascending)
1.0	Ozone for 3 lowest layers deviates from climatology; probable volcanic contamination (ascending)
2.0	Profile total ozone inconsistent with best ozone from total ozone algorithm (ascending)

Profile Error Code	Description
3.0	Large final residue (ascending)
4.0	Initial residue > 60% (ascending)
5.0	C outside 0.5-3.0 mbar (ascending)
6.0	σ outside 0.3-0.8 mbar (ascending)
7.0	Reflectivity outside range –0.05 to 1.05, or changes by more than 0.15 (ascending)
8.0	No best total ozone available (ascending)
9.0	Bad counts or missing measurements (ascending)
10.0	Good profile (descending)
11.0	Ozone for 3 lowest layers deviates from climatology; probable volcanic contamination (descending)
12.0	Profile total ozone inconsistent with best ozone from total ozone algorithm (descending)
13.0	Large final residue (descending)
14.0	Initial residue > 60% (descending)
15.0	C outside 0.5-3.0 mbar (descending)
16.0	σ outside 0.3-0.8 mbar (descending)
17.0	Reflectivity outside range –0.05 to 1.05, or changes by more than 0.15 (descending)
18.0	No best total ozone available (descending)
19.0	Bad counts or missing measurements (descending)
20.0	Inputs to the algorithm were detected to be invalid or out of range

2.1.5 Data Quality Monitoring

Each algorithm uses specific criteria contained in a Data Quality Threshold Table (DQTT) to determine when a Data Quality Notification (DQN) is produced. The DQTT contains the threshold used to trigger the DQN as well as the text contained in the DQN. If a threshold is met, the algorithm stores a DQN in DMS indicating the test(s) that failed and the value of the DQN attribute. For more algorithm specific detail refer to the CDFCB-X.

2.1.6 Computational Precision Requirements

The OMPS NP (SBUV/2 V6) algorithm is based on an older heritage algorithm. It is coded to use ‘real’ and ‘integer’ declared variables. Double precision real variables or long integers are therefore not required for computational accuracy.

2.1.7 Algorithm Support Considerations

2.1.7.1 Numerical Computation Considerations

The NP retrieval algorithm is not computationally intensive. Double precision computations are not required. In fitpro.f, calls to spline() and splint() from Numerical Recipes have been replaced with cubspl() from pppack and with cubsplint(), respectively.

2.1.7.2 Software Environment Considerations

The DMS and INF subsystems must be running before the algorithm is executed. Fortran 90 and C++ compilers are needed to compile the NP IP algorithm.

2.1.7.3 Future Development

The algorithm, at some future time, should be upgraded to use hyperspectral information provided by the NP sensor. The NP algorithm should make use of other EDR information rather than static climatological databases. For example, the algorithm could make use of VIIRS cloud pressure data and CrIS terrain pressure, which would enable more accurate calculations. Replacing the NP algorithm, which is the SBUV/2 Version 6 with the SBUV/2 Version 8 algorithm, should also be considered.

2.1.8 Assumptions and Limitations

2.1.8.1 Assumptions

All necessary data is available and provided within the necessary time constraints.

2.1.8.2 Limitations

None

2.2 OMPS Nadir Profile Version 8 IP Description

2.2.1 Interfaces

The NP V8Pro IP algorithm is initiated in the same way as the NP V6Pro IP as it is a follow-on process.

2.2.1.1 Inputs

The NP V8Pro IP science processing requires the PMF record (described in Section 2.1.1.1 and Table 3, with entries indicated as "V8Pro use" as input for this algorithm and other values just passed through to the output). It also requires an additional set of inputs. The input for the OMPS instruments has the same types of input data as the V8 SBUV but the OMPS input data has been merged into a single input file named OMPS-NP-LUT.. It has all the components as listed in section 1.1. There is an XML document that describes each component of the OMPS-NP-LUT file named OMPS_NP_LUT.xml.

2.2.1.1.1 Look-Up Tables

The V8Pro processor utilizes look-up tables. Files derived from the SBUV2 implementation in the offline Fortran code were merged into a single LUT file by appending them to the current V6Pro LUT. For details see the corresponding XML description of the updated IP OMPS-NP-LUT**.** The description of the files is included below.

Besides the input observations from V6Pro PMF data file, V8Pro processing system also accesses multiple auxiliary input data sets.

Constants

> This file is in ASCII format and contains instrument calibration and algorithm constant parameters. A brief description to each line of data has been given in the file.

N-value look-up tables

> This file is in sequential binary format consisting of 13 records of data, each of which contains four look-up tables for one grating position offset. The four look-up tables are for calculating total intensity due to the atmospheric backscatter, single scattering intensity due to the atmospheric backscatter, transmittance for ground reflected radiation and average of fraction of radiation scattered back from the atmosphere, respectively. All these tables except the last one have dimensionality of (10, 21, 9, 4) corresponding to (solar zenith angle, profile, wavelength, pressure). The last table is not dependent on solar zenith angle, thus has dimension (21, 9, 4).
>
> This constant data file is instrument dependent, a dedicated file must be provided for each satellite or instrument.

N-value sensitivity look-up tables

> This file is in sequential binary format consisting of only one record of data, which contains four look-up tables for calculating N-value sensitivity. The four look-up tables are same as those for N-value except additional dimension of 12 is added for the

unperturbed case followed by 11 cases perturbed in Umkehr layer 0-9 and 10, 11 and 12 combined.

This constant data file is instrument dependent, a dedicated file must be provided for each satellite or instrument.

A priori ozone profile climatology

This file is in sequential binary format consisting of only one record of data, which contains a priori ozone profiles in 13 Umkehr layers (12-0) for 18 10-degree latitude zones (from south to north) and 12 months from January to December.

A priori temperature profile climatology

This file is in sequential binary format consisting of only one record of data, which contains a priori temperature profiles in 13 Umkehr layers (12-0) for 18 10-degree latitude zones (from south to north) and 12 months from January to December.

Standard profiles in fine layers

This file is in ASCII format and contains one standard temperature and 21 ozone profiles (3 for low latitude with total ozone from 225 to 325 DU; 8 for mid latitude with total ozone from 225 to 575 DU; and 10 for high latitude with total ozone from 125 to 575 DU) in 81 layers. The profile data consisting of 81 records, one for each layer, start from the third record. The records have format of (f9.6, f7.2, 21f10.6), corresponding to 1 scaled pressure (0 for the top of the atmosphere and 1 for the ground), 1 temperature and 21 layer ozone amounts.

Solar radiation reference look-up table

This file is in ASCII format and contains solar radiation reference data with high wavelength resolution (~0.05 nm). Each record is for one wavelength, including 7 parameters, i.e., wavelength, 3 ozone absorption coefficients, Rayleigh scattering coefficient, molecular anisotropy and solar flux.

Terrain height pressure data

This file is in sequential binary format consisting of only one record of data, which contains 0.5 degree resolution terrain height pressure data with dimension (360, 720).

Surface category code

This file is in ASCII format consisting of 2160 records with 120 characters per record, which corresponds to a (360, 720) array of 0.5 degree resolution surface category codes (every 6 records hold data for one latitude zone). Only 0, 1 and 2 are possible in the file, representing ocean, land and low inland water body, respectively.

Snow-ice cover data

There are 12 snow-ice cover data files in total, one for each month. These files are in ASCII format consisting of 3600 records with 18 floating point numbers per record, corresponding to a (180, 360) array of 1 degree resolution snow-ice cover data (every 20 records hold data for one latitude zone).

Cloud pressure data

There are totally 12 cloud pressure data files, one for each month. These files are in ASCII format consisting of 3600 records with 18 floating point numbers per record, corresponding to a (180, 360) array of 1 degree resolution cloud pressure data (every 20 records hold data for one latitude zone).

Merged a priori ozone climatology

This file is in ASCII format consisting of 2160 (10 total ozone amounts * 18 latitude zones * 12 months) climatological 11-layer ozone profiles. The file is organized as a sequence of profile data blocks. Each block consists of a header record with month and latitude zone information and 10 data records of 12 floating point numbers. The first number represents the total ozone amount of the profile, ranging from 125 to 575 DU, followed by 11 layer ozone values.

The V8Pro input is appended to then end of the V6Pro file. The content listed in the table below.

Table 10. Nadir Profile V8PRO IP LUT

Parameter	Dimension	Description	Units
CLIMOZ	real(13,18,12)	Ozone Profile Climatology for a priori	DU
CLIMTM	real(13,18,12)	Temperature Profile Climatology	Kelvin
OZP81	real(81,21)	81-layer standard profiles	DU
TZAPRF	real(11,10,18,13)	11-layer profile for total ozone	DU
WLENTH	real(13)	Measurement Wavelengths	nm
FWHM	real(13)	Bandpass Full width Half Maximum	nm
COV_WEIGHT	real(13)	Flag used to disable the measurement process of any channel	
NVALADJ	real(13)	Soft Calibration Adjustment	N-value
REF_WLENTH	real(2023)	Absorption parameter wavelength	Angstrom
A0	real(2023)	Ozone Absorption constant parameter	$(atm\text{-}cm)^{-1}$
A1	real(2023)	Ozone Absorption linear parameter	$(atm\text{-}cm)^{-1}K^{-1}$
A2	real(2023)	Ozone Absorption quadratic parameter	$(atm\text{-}cm)^{-1}K^{-2}$
B	real(2023)	Rayleigh Scattering	atm^{-1}
RHO	real(2023)	Anisotropy	
FLUX	real(2023)	Solar Flux	
LOGI0_V8	real(10,21,9,4)	Log I0	Unitless
TTI0_V8	real(10,21,9,4)	Downward transmission	Unitless
SB_V8	real(21,9,4)	Surface backscatter fractions	Unitless
LOGI0SS_V8	real(10,21,9,4)	Single Scattering component of Log IO	Unitless
LOGI0_DNDX	real(10,21,9,4,12)	Layer sensitivities of Log I0	DU^{-1}
TTI0_DNDX	real(10,21,9,4,12)	Layer sensitivities of Downward transmission	DU^{-1}

SB_DNDX	real(21,9,4,12)	Layer sensitivities of Surface backscatter fractions	DU^{-1}
LOGI0SS_DNDX	real(10,21,9,4,12)	Layer sensitivities of Single Scattering component of Log IO	DU^{-1}
CLOUD_PRESS	real(360,180,12)	UV Cloud Top Optical Centroid Climatology	Atm.
SNOW_ICE_MAP	real(360,180,12)	Snow Ice Climatology	Percent
PS	real(360,720)	Terrain Height Pressure	Atm.
CAT	real(360,720)	Surface Category	0, 1, or 2
RAMCOR	real(9,6)	Raman Correction Coefficients	N-value

2.2.1.2 Outputs

The V8Pro IP outputs are included in the new IMOPO output file. The total content is described in the table below and in the text following it.

Table 11. Ozone Nadir Profile IP Data Content Summary

Name	Description	Data Type	Aggregate Dimensions (N=Number of Granules)	Granule Dimensions	Units
NormalizedRadiance_380nm	Normalized radiance value for 380 nm wavelength	32-bit floating point	[N*1, 1]	[1, 1]	N Value
NormalizedRadiance_340nm_331nm_318nm_312nm	Total column sensor N values for the 340, 331, 318, and 312 nm channels	32-bit floating point	[N*1, 1, 4]	[1, 1, 4]	N Value
Wavelengths	13 Wavelengths of Observation	32-bit floating point	[N*1,1,13]	[1,1,13]	nm
A-PairTotalO3	Total ozone amount derived from the A-pair of wavelengths	32-bit floating point	[N*1, 1]	[1, 1]	milli-atm-cm (DU)
A-PairSensitivity	A pair sensitivity	32-bit floating point	[N*1, 1]	[1, 1]	(N-Value)/DU
A-PairReflectivity	A pair average reflectivity	32-bit floating point	[N*1, 1]	[1, 1]	percent
A-PairWeight	A pair weight (weighting factor in TOZ calc)	32-bit floating point	[N*1, 1]	[1, 1]	unitless
B-PairTotalO3	Total ozone amount derived from the B-pair of wavelengths	32-bit floating point	[N*1, 1]	[1, 1]	milli-atm-cm (DU)
B-PairSensitivity	B pair sensitivity	32-bit floating point	[N*1, 1]	[1, 1]	(N-Value)/DU
B-PairReflectivity	B pair average reflectivity	32-bit floating point	[N*1, 1]	[1, 1]	percent
B-PairWeight	B pair weight (weighting factor in TOZ calc)	32-bit floating point	[N*1, 1]	[1, 1]	unitless
ColumnAmountO3	Best estimate total ozone	32-bit floating point	[N*1, 1]	[1, 1]	DU
C-PairTotalO3	Total ozone amount derived from the C-pair of wavelengths	32-bit floating point	[N*1, 1]	[1, 1]	milli-atm-cm (DU)
ReflSurfPressure	Pressure of reflecting surface	32-bit floating point	[N*1, 1]	[1, 1]	Atm
BestReflectivity	Best Reflectivity from retrieval	32-bit floating point	[N*1, 1]	[1, 1]	percent
C-PairSensitivity	C pair sensitivity	32-bit floating point	[N*1, 1]	[1, 1]	(N-Value)/DU
OzoneErrorFlagforBestOzone	Ozone Error Flag for Best Ozone - indicates error in	32-bit floating point	[N*1, 1]	[1, 1]	unitless

Name	Description	Data Type	Aggregate Dimensions (N=Number of Granules)	Granule Dimensions	Units
	retrieval Values range from 0 - 20				
tableIndex	Table Selection Index 0 - Low Latitude; 1 - Mid Latitude; 2 - High Latitude	32-bit floating point	[N*1, 1]	[1, 1]	unitless
SnowIceCode	Snow/Ice Code	32-bit floating point	[N*1, 1]	[1, 1]	unitless
TerrainPressure	Terrain (ground) pressure	32-bit floating point	[N*1, 1]	[1, 1]	Atm
D-PairTotalO3	Total ozone amount derived from the D-pair of wavelengths	32-bit floating point	[N*1, 1]	[1, 1]	milli-atm-cm (DU)
SO2index	Sulfur Dioxide Index	32-bit floating point	[N*1, 1]	[1, 1]	unitless
BPrime-PairTotalO3	Total ozone amount derived from the B Prime Pair of wavelengths	32-bit floating point	[N*1, 1]	[1, 1]	milli-atm-cm (DU)
N_Values_InterpolatedToSBUVmon	N values interpolated from the radiances from the 147 wavelengths of the NP sensor to the SBUV/2 profiling wavelengths (for SBUV/2 were the n-values of the profiling wavelengths)	32-bit floating point	[N*1, 1, 8]	[1, 1, 8]	N Value
FirstGuessO3Profile	First guess profile for layers	32-bit floating point	[N*1, 1, 12]	[1, 1, 12]	milli-atm-cm (DU)
FirstGuessTotalO3	Total ozone for first guess	32-bit floating point	[N*1, 1]	[1, 1]	milli-atm-cm (DU)
QValues	Q-Value corrected for multiple scattering and surface reflectivity (listed in order from shorter to longer wavelengths … 255.5 to 317.5 nm)	32-bit floating point	[N*1, 1, 10]	[1, 1, 10]	unitless
InitialResiduals	Initial residues of Q-Values	32-bit floating point	[N*1, 1, 10]	[1, 1, 10]	percent
QValuesCorrectionsLonger	Correction to Q-Values (pressure levels) for the five longer wavelength channels due to Multiple Scattering and Reflectivity (MSR); Listed from shorter to longer wavelength	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	unitless
ReflectivitiesLonger	Monochromator reflectivities for the five longer wavelengths; Listed from shorter to longer wavelength (297.5nm to 317.5nm)	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	percent
MultipleScatteringSensitivity	Multiple scattering sensitivity for five longer wavelengths (297.5 to 317.5 nm)	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	Q value)/DU
MultipleScatteringMix	Multiple scattering mixing fraction - The mixing fraction which parameterizes	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	unitless

Name	Description	Data Type	Aggregate Dimensions (N=Number of Granules)	Granule Dimensions	Units
	contributions of lower and higher latitude profiles in determination of MSR radiance from lookup tables				
FinalQValueResidues	Final residues of Q-Values (percent) derived using obtained from final solution profile; Listed from shorter to longer wavelength (255.5nm to 317.5nm)	32-bit floating point	[N*1, 1, 10]	[1, 1, 10]	percent
FinalO3Profile	Solution profile individual ozone amounts (matm-cm) in 12 SBUV layers (SBUV layer 1 first)	32-bit floating point	[N*1, 1, 12]	[1, 1, 12]	milli-atm-cm (DU)
FinalO3Profile_Std	Standard deviations for solution profile individual ozone amounts (%) in 12 SBUV layers	32-bit floating point	[N*1, 1, 12]	[1, 1, 12]	percent
TotalO3SolutionProfile	Total ozone for solution profile (above 1 atm)	32-bit floating point	[N*1, 1]	[1, 1]	milli-atm-cm (DU)
OzoneErrorFlagforProfile	Ozone Error Flag for Profile 0 - Good Profile (Ascending) 10 - Good Profile (Descending)	32-bit floating point	[N*1, 1]	[1, 1]	unitless
CParameter	C parameter for c-sigma calculation. Represents the ratio of atmospheric scale height to the ozone scale height in C-Sigma validity check; Sigma should range from 0.3 to 0.8 or an error code is assigned.	32-bit floating point	[N*1, 1]	[1, 1]	unitless
SigmaParameter	Sigma parameter for c-sigma calculation. Represents the ratio of atmospheric scale height to the ozone scale height in C-Sigma validity check; Sigma should range from 0.3 to 0.8 or an error code is assigned.	32-bit floating point	[N*1, 1]	[1, 1]	unitless
O3MixingRatio	Volume mixing ratio (from spline interpolation) of ozone at 19 pressure levels in order of increasing atmospheric pressure (0.3 mb to 100 mb)	32-bit floating point	[N*1, 1, 19]	[1, 1, 19]	ppmv
FirstGuessO3_Std	Standard deviations of first guess (a priori) profile individual ozone amounts (%) in 12 layers (SBUV	32-bit floating point	[N*1, 1, 12]	[1, 1, 12]	percent

Name	Description	Data Type	Aggregate Dimensions (N=Number of Granules)	Granule Dimensions	Units
	layer 1 first)				
QValues_Std	Standard deviations for Q-values corrected for multiple scattering and reflectivity (255.5 nm through 317.5 nm) in %	32-bit floating point	[N*1, 1, 10]	[1, 1, 10]	unitless
Iterations	Number of iterations for profile solution	32-bit floating point	[N*1, 1]	[1, 1]	unitless
VolcanoContaminationIdx	Volcano Contamination Index (VCI): Can be used to whether the derived profiles below 5 mb are incorrect because of scattering by aerosols. VCI are in units of the climatological standard deviation of the tropospheric ozone value for a given latitude.	32-bit floating point	[N*1, 1]	[1, 1]	unitless
D-PairSensitivity	D pair sensitivity	32-bit floating point	[N*1, 1]	[1, 1]	(N-Value)/DU
BPrime-PairSensitivity	B Prime pair sensitivity	32-bit floating point	[N*1, 1]	[1, 1]	(N-Value)/DU
SAA	Spacecraft within South Atlantic Anomaly (extent in percent based on Climatological data)	unsigned 8-bit char	[N*1]	[1]	unitless
SunGlint	Sun glint indication (scattering angle and surface type thresholds)	unsigned 8-bit char	[N*1, 1]	[1, 1]	unitless
SolarEclipse	All or part of the IFOV is affected by a solar eclipse, umbra or penumbra viewing.	unsigned 8-bit char	[N*1, 1]	[1, 1]	unitless
Implicit_pad0	Pad byte	unsigned 8-bit char	[N*1, 1]	[1, 1]	unitless
FinalO3ProfileV8	21 layer ozone profile retrieval	32-bit floating point	[N*1, 1]	[1, 1, 21]	DU
Step1O3_v8	Step 1 total column ozone	32-bit floating point	[N*1, 1]	[1, 1]	DU
Step2O3_v8	Step 2 total column ozone	32-bit floating point	[N*1, 1]	[1, 1]	DU
bestozone_v8	Final ozone estimate from the V8 total ozone calculation	32-bit floating point	[N*1, 1]	[1, 1]	DU
cloudfrac_v8	V8 Cloud Fraction	32-bit floating point	[N*1, 1]	[1, 1]	unitless
errflag_v8	V8 Error Flag total ozone	32-bit integer	[N*1, 1]	[1, 1]	unitless
algflag_v8	Total Ozone Algorithm Flag	32-bit integer	[N*1, 1]	[1, 1]	unitless
cloudpres_v8	Cloud Top Pressure: Atmospheres	32-bit floating point	[N*1, 1]	[1, 1]	atmospheres
groundpres_v8	Surface pressure, atmospheres	32-bit floating point	[N*1, 1]	[1, 1]	atmospheres
ref331_v8	Effective reflectivity from 331 nm	32-bit floating point	[N*1, 1]	[1, 1]	unitless
ref360_v8	Effective reflectivity from 360 nm	32-bit floating point	[N*1, 1]	[1, 1]	unitless
dn360_v8	N-value change for reflectivity	32-bit floating point	[N*1, 1]	[1, 1]	nvalue

Name	Description	Data Type	Aggregate Dimensions (N=Number of Granules)	Granule Dimensions	Units
aerind_v8	UV Aerosol Index	32-bit floating point	[N*1, 1]	[1, 1]	unitless
ozcloud_v8	Ozone below cloud	32-bit floating point	[N*1, 1]	[1, 1]	DU
sens_v8	dN/dOmega for total ozone channels	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	unitless
resn_v8	Residuals for the total ozone channels from the total ozone retrieval, N-values	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	n-values
dndr_v8	N-Value sensitivities for five total ozone channels; N-values per reflectivity unit	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	n-values per reflectivity
toz_apprf_v8	11-layer profile for total ozone	32-bit floating point	[N*1, 1, 11]	[1, 1, 11]	DU
efficiency_v8	Layer retrieval efficiency	32-bit floating point	[N*1, 1, 11]	[1, 1, 11]	DU/DU
niteration_v8	Number of iterations of the linearized optimal estimation	32-bit integer	[N*1, 1]	[1, 1]	unitless
profile_code_v8	V8 error code ozone profile	32-bit integer	[N*1, 1]	[1, 1]	unitless
tozpro_v8	Profile total, 0 to 900	32-bit floating point	[N*1, 1]	[1, 1]	DU
resqc_v8	Quality control residual for total ozone	32-bit floating point	[N*1, 1]	[1, 1]	unitless
mixing_ratio_v8	Ozone mixing ratios at 15 pressure levels	32-bit floating point	[N*1, 1, 15]	[1, 1, 15]	VMR
mixing_ratio_err_v8	Estimated 1 sigma errors for mixing ratios.	32-bit floating point	[N*1, 1, 15]	[1, 1, 15]	ppmv
mixing_ratio_press_v8	15 Pressure levels for mixing ratios	32-bit floating point	[N*1, 1, 15]	[1, 1, 15]	hPa
residual_v8	Final residuals for ten shortest wavelengths for the profile retrieval	32-bit floating point	[N*1, 1, 10]	[1, 1, 10]	nvalue
residual0_v8	Initial residuals for ten shortest wavelengths	32-bit floating point	[N*1, 1, 10]	[1, 1, 10]	nvalue
profile_firstguess_v8	21 layer First guess ozone profile	32-bit floating point	[N*1, 1, 21]	[1, 1, 21]	DU
profile_apriori_v8	21 Layer ozone a priori profile	32-bit floating point	[N*1, 1, 21]	[1, 1, 21]	DU
profile_temperature_v8	21 layer temperature profile	32-bit floating point	[N*1, 1, 21]	[1, 1, 21]	Kelvin
averaging_kernel_v8	Averaging Kernel	32-bit floating point	[N*1, 1, 20, 20]	[1, 1, 20, 20]	unitless
snow_ice_v8	Snow/ice coverage	32-bit integer	[N*1, 1]	[1, 1]	Percent
sza_v8	Solar Zenith Angle at FOV center	32-bit floating point	[N*1, 1]	[1, 1]	Degree
longitude_v8	Longitude for middle and four corners	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	Degree
latitude_v8	Latitude for middle and four corners	32-bit floating point	[N*1, 1, 5]	[1, 1, 5]	Degree
Jacobian	Jacobian of partial derivatives of radiances at ten channels with respect to 20 ozone layer amounts	32-bit floating point	[N*1, 1, 10, 20]	[1, 1, 10, 20]	unitless
File Size	3992 Bytes				

Table 12. V8Pro Total Ozone Error Code and Descriptions

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

Table 13. V8Pro Profile Error Code and Descriptions

Profile Error Code	Description
0.0	Good retrieval
1.0	SZA > 84 degrees
2.0	|Step3O3 – Profile Total| > 25 DU
3.0	Average |Final Residual| for retrieval channels > threshold
4.0	|Final residue| greater than 3 times instrument error
5.0	|Retrieved - a priori| greater than 3 times a priori error
6.0	Non-convergent solution
7.0	Stray light anomaly
8.0	Initial residue greater than 18.0 N-value units or upper level profile anomaly
9.0	Total ozone algorithm failure
+10.0	10 is added - to the flag values to designate descending portions of the orbit. The unit's value is unchanged.

2.2.2 Algorithm Processing

At the point where original IMOPO science source code finished an additional call is now made. The algorithm computes and populates additional data fields. The new code computes the o3prov8 solution ozone profile and diagnostics. These are placed in memory. The science code ends and control returns to the PRO driver where the science code solution profile data is further processed.

The OMPS Version 8 algorithm works as a follow-on processing system to the existing Version 6 algorithm and uses the Version 6 output as input. Functionally, the Version 8 processing system can be divided into three main parts: job initialization, total ozone retrieval and profile ozone retrieval. In the initialization part look-up tables for radiative transfer calculations and a priori ozone and temperature climatological data sets are read in and various parameters and coefficients are determined. Step by step summaries for these three parts are given in the following sections. Some nonessential details may be omitted.

The Flow Charts (Figure 5, Figure 6, Figure 7 and Figure 8) are provided in Appendix A.

A. Initialization (START Flow Figure 6)

The subroutine performs the following job initialization tasks:

i. Initializes the ancillary data needed for the algorithm. This includes:
- N-value look-up tables as functions of 4 pressure levels, 9 channels, 21 profiles and 10 solar zenith angles.
- Sensitivity dN/dX_{msr} look-up tables as functions of 4 pressure levels, 9 channels, 21 profiles, 10 solar zenith angles and 12 perturbation situations (unperturbed case followed by 11 Umkehr layers' perturbation).
- 21 standard profiles in 81 layers.
- Merged a priori 11-layer ozone profile climatology as function of 10 total ozone values, 18 latitude zones and 12 months.
- A priori 13-layer ozone profile climatology as function of 18 latitude zones and 12 months.
- A priori 13-layer temperature climatology as function of 18 latitude zones and 12 months.

ii. Calls READ_CLIM, RDCONS, CNSTNTS, READ_MSR_TABLES, INIT_DNDT and INIT_DNDT_TOZ to initialize various parameters used in total and profile ozone retrievals. These include temperature dependent coefficients of absorption coefficient, denominators of Lagrangian coefficients for solar zenith angle and pressure interpolations, and radiance measurement error covariance matrix. The subroutine COFFS is called by CNSTNTS to assign component wavelengths within each SBUV channel, determines ozone absorption coefficients, Rayleigh scattering coefficients, and phase function coefficients at those wavelengths, and also determines the weights of the components for computation of the average channel intensity.

B Total ozone retrieval (TOTAL_V8 Flow Figure 7)

The Version 8 SBUV operational system adopts the total column ozone retrieval algorithm developed for TOMS instruments (*Bhartia and Wellemeyer, 2004*), though necessary modifications have been made to fit SBUV instruments. The retrieval algorithm is a three-step process of successive estimation improvement. Step 1) the algorithm uses a pair of wavelengths 331 nm and 318 nm (340 nm and 331 nm for high solar zenith angle) to derive reflectivity and total ozone as a first guess linearization point. Step 2) adjustments due to seasonal and latitudinal variations in ozone and temperature profiles are made. Step 3) a simple procedure based on N-value residues is followed to correct errors due to aerosol, sea glint and profile shape deviation.

i. Calls SCANINV8 to perform initialization tasks for a single SBUV total and profile ozone retrievals:
   1) Sets latitude flag for table look-up: ILAT=1 [0, 30]; 2 (30, 60] or 3 (60, 90].
   2) Calls subroutine INTER to read in 0.5 degree resolution terrain height pressure and surface category and 1 degree resolution snow-ice thickness and cloud top pressure fields. Interpolate these climatological data for the date, latitude and longitude of the observation.
   3) Determines solar zenith angle for each wavelength channel.
   4) Computes Lagrange coefficients for solar zenith angle interpolation.

ii. Detects wild radiances and skip the retrieval for bad observations.

iii. Assumes a nominal total ozone amount according to the latitude of observation: GUESOZ = 260 [0, 45]; 340 (45, 75] or 360 (75, 90].

iv. Calls REFLECV8 to calculate total ozone sensitivity at 340 nm wavelength channel:
   1) Coverts the reflectivity channel N-value to albedos.
   2) Initializes ground and cloud reflectivities to 0.15 and 0.80, respectively, at the first time routine call.

3) Perturbs measured reflectivity channel N-value by 0.2%.
4) Calls PRFIND to determine indices of bracketing standard ozone profiles based on total ozone estimation and latitude flag ILAT at the first time routine call.
5) For each of the bracketing ozone profiles, calls IZTRSB to perform look-up table pressure interpolations for i_0, T_r and s_b, and then calculates radiance from ground and cloud.
6) Computes terrain height corrections to the total ozone of bracketing profiles and bracketing interpolation coefficient.
7) Calls GETRNG to calculate Raman corrections
8) Interpolates logarithm of table parameters to current total ozone estimate and converts to ground and cloud radiances.
9) Calculates cloud fractions for unperturbed and perturbed cases. Assumes clear sky if snow is present.
10) Calculates reflectivities for both unperturbed and perturbed cases: if the cloud fraction is less than or equal to 0.0 or greater than or equal to 1.0, then the reflectivity is calculated using table parameters interpolated to the appropriate pressure level as

$$R = \frac{1}{\frac{T_r}{I_m - I_0} + s_b}$$

If the cloud fraction is greater than 0.0 and less than 1.0, then the reflectivity is

$$R = R_g + f_c * (R_c - R_g)$$

Total ozone sensitivity is calculated during the first call of the REFLECV8 routine.

v. Calls REFLECV8 to calculate cloud fraction, reflectivity and total ozone sensitivity at reflectivity channel (see above).

vi. Call REFL_360 to calculate cloud fraction and reflectivity for each scene from the photometer measurements. Do reflectivity channel first as a reference. Detailed descriptions are omitted here.

1) Converts photometer N-value to albedos.
2) Initialize ground and cloud reflectivities with ones from monochromator reflectivity channel.
3) Perturbs measured photometer N-value at the reflectivity channel by 0.2%.
4) For each of the bracketing ozone profiles, calls IZTRSB to perform look-up table pressure interpolations for i_0, T_r and s_b, and then calculates radiance from ground and cloud.
5) Computes terrain height corrections to the total ozone of bracketing profiles and bracketing interpolation coefficient.
6) Calls GETRNG to calculate Raman corrections
7) Interpolates logarithm of table parameters to current total ozone estimate and converts to ground and cloud radiances
8) Calculates cloud fractions for unperturbed and perturbed cases. Assumes clear sky if snow is present.
9) Calculates reflectivities for both unperturbed and perturbed cases: if the cloud fraction is less than or equal to 0.0 or greater than or equal to 1.0, then the

reflectivity is calculated using table parameters interpolated to the appropriate pressure level as

$$R = \frac{1}{\frac{T_r}{I_m - I_0} + s_b}$$

If the cloud fraction is greater than 0.0 and less than 1.0, then the reflectivity is

$$R = R_g + f_c * (R_c - R_g)$$

Total ozone sensitivity is calculated during the first call of the REFLECV8 routine.

10) Calculates residue and reflectivity sensitivity at reflectivity channel.
11) Recalculates surface model parameters based on CCR reflectivity

vii. Calls OZNOT to compute initial total ozone estimate using implied ozone channel (318 nm for regular and 331 nm for some extreme cases. See step viii.)

1) For the first call to OZNOT the iterative technique is used to find total ozone amounts that provide table N-value that bracket the measured N-value:
   a. For current ozone index, calls IZTRSB to calculate look-up table parameters i_0, T_r and s_b.
   b. Calls GETRNG to calculate Raman corrections.
   c. Determines calculated N-value for ozone wavelength channel
   d. Calls NVBRAC to determine whether the N-value for the current ozone index is above, below, or completes a bracketing of the measured N-value. If bracketing is not complete, repeats steps a-d until it is.
2) On subsequent calls to OZNOT, the bracketing profiles determined in the first call are retained even if extrapolation is required. For each of the two bracketing ozone profiles:
   a. Calls IZTRSB to calculate look-up table parameters i_0, T_r and s_b.
   b. Calls GETRNG to calculate Raman corrections.
   c. Determines calculated N-value for ozone wavelength channel
3) For all calls to OZNOT, estimates total ozone using the local slope of the N-Ω curve, $dN/d\Omega$ as

$$\Omega = \Omega_1 + (N_m - N_1)/(dN/d\Omega)$$

viii. After the first iteration, if

$$\frac{\frac{dN}{d\Omega_{318}} - \frac{dN}{d\Omega_{331}}}{\frac{dN}{d\Omega_{331}} - \frac{dN}{d\Omega_{340}}} < 1.25$$

then resets for computing total ozone using C pair (331 nm and 340 nm) in stead of B pair (318 nm and 331 nm) and start over from Step v.

ix. Iterates Step v-vii until the updated ozone estimate changes by less than 1.0 DU.

x. Calls RESIDUE to compute N-value residue for each of the multiple scattered wavelengths:

1) Calls IZTRSB to compute look-up table parameters i_0, T_r and s_b for bracketing profiles.
2) Calculates terrain adjusted bracketing total ozone amounts and ozone interpolation coefficient.

3) Calls GETRNG to calculate Raman corrections.
4) Calculates N-values for unperturbed and perturbed reflectivities.
5) Computes N-value residues, ozone sensitivities and reflectivity sensitivities.
6) Adjust observed N-values with Raman correction for profile retrieval

xi. Calls GETMSR to compute multiple scattered and surface reflected part of the Jacobian dN / dX for each of 11 Umkehr layers and each of 8 wavelengths using finite differencing between N-values interpolated from unperturbed and perturbed ozone tables.
1) Calls SBDNDX to perform table lookups for computation of dN / dX .
2) Calculates radiance from ground and cloud top for 12 layers (1 unperturbed followed by 11 with perturbations in 11 Umkehr layers) and 4 pressure levels.
3) Performs pressure interpolations through function PINTRP.
4) Combines ground and cloud radiances according to cloud fraction.
5) Calculates N-value perturbations and unperturbed N-values.
6) For perturbed layers, computes layer sensitivities for total, SS and MSR. Assigns MSR kernel as MSR sensitivities.
7) For the unperturbed case, computes multiple scattered and reflected part of total radiance.

xii. Calls APRSBO to determine 13-layer a priori ozone profile and integrated total ozone for the day and latitude.

xiii. Calls APRSBT to determine 13-layer a priori temperature profile for the day and latitude.

xiv. Defines 11-layer a priori temperature profile from 13-layer profile.

xv. Calls STNP81 to determine 81-layer first guess ozone profile for profile retrieval.

xvi. Calls DN_BY_DT to compute MSR dN due to temperature difference for MSR radiances each of 11 Umkehr layers and each of 8 wavelengths using chain rule relating dN / dT to dN / dX

xvii. Adjusts MSR radiances for a priori temperature profile.

xviii. Calls GETSHP to determine merged a priori ozone profile given total ozone, day of year and latitude.

xix. Calls DN_BY_DT to determine temperature adjustments again for dN / dX .

xx. Calls OZONE_V8 to calculate Step 2 total ozone, which improves the Step 1 total ozone based on a priori information about the seasonal and latitudinal variations in ozone profile shape and in temperature. The solution profile is adjusted due to the change in total ozone for estimation of column ozone below the cloud.

xxi. Calls RESADJ to adjust N-value residues after calculation of the Step 2 total ozone.

xxii. Computes Step 3 total ozone There are three possible corrections:
- A correction for the impact of tropospheric aerosol and sun glint with photometer residue at reflectivity channel.
- A correction with 313 nm wavelength N-value residue for the deviations of the true vertical distribution of ozone relative to the a priori climatology assumed in step 2
- A correction for non-zero N-value residues at ozone and reflectivity channels if C-pair is used.

xxiii. Calls BLWCLD to calculate column ozone below the cloud layer.

xxiv. Calls SETERR to set error flags.

C. Ozone profile retrieval (PROFILE_V8 Flow Figure 8)

The inverse problem of deriving an ozone profile from SBUV measurements is mathematically ill-posed, some kind of constrain must be applied in order to achieve a physically reasonable solution. Based on the optimal estimation technique (*Rodgers, 1990*), the version 8 SBUV ozone profile retrieval algorithm combines SBUV measurements and a priori profile information to achieve the maximum likelihood estimate. The solution of the ozone profile is achieved through an iteration procedure following the equation:

$$q_{n+1} = q_a + S_a * K_n^T * (K_n * S_a * K_n^T + S_e)^{-1} * ((N - F(q_n)) + K_n * (q_n - q_a))$$

where $n+1$ and n refer to the current and previous iterations, q is the ozone profile vector, N is the N-value measurement vector, q_a is the a priori ozone profile vector, $F(q)$ is the forward model simulating N, K is the kernel (dF/dq), S_e and S_a are the measurement and a priori profile covariance matrices, respectively.

Ozone amounts in the top layers are assumed to be distributed according to the power law: q proportional to $p^{1/\sigma}$, with σ determined from several layers below the topmost layer.

The profile retrieval is carried out in fine (81) layers and converted to coarse (21) layers for output.

i. Calls INTERPOL_QO3 to interpolate a priori ozone profile from 13 Umkehr layers to 81 fine layers.
ii. Calls INTERPOL_T to interpolate a priori temperature profile from 13 Umkehr layers to 81 fine layer s
iii. Calls INTERPOL_KERN to interpolate multiple scattered kernels to 81 fine layers for clear and cloud cases separately, and then calculates the MSR kernel as a weighted average of clear and cloud kernels according to the cloud fraction.
iv. Defines a priori covariance matrix S_a.
v. Calls O3_RETRIEVAL to retrieve ozone profile using Rodgers method.
    1) Calls O3_SNGLSCATT to run single scattering forward model to estimate radiance and kernel.
    2) Computes single scattering radiances and kernels at cloud and terrain levels and combine according to the cloud fraction.
    3) Converts single scattering radiance and kernel into N-value and dN/dX.
    4) Adds multiple scattering contributions to N-value and kernel.
    5) Defines aerosol related processing algorithm, i.e., includes measurements only from channels up to where the kernel for a layer near 100 hPa is maximum by assigning S_e for longer wavelength channels to a very large value.
    6) Computes N-value residues and exit loop if desired limit is attained.
    7) Calls UPDATE to update ozone profile using Rodgers' method:
        a. Computes $K_{aux} = K_n * S_a$.
        b. Computes $S_{aux} = K_{aux} * K_n^T + S_e$.
        c. Calls FACTOR to perform LU factorization of S_{aux}.
        d. Computes mismatches $diff = (N - F(q_n)) + K_n * (q_n - q_a)$.
        e. Calls INVERSE to compute $S^{-1}{}_{aux} * diff$

f. Updates ozone profile $q_{n+1} = q_n + K_{aux}^T * S_{aux}^{-1} * diff$

8) Performs linear fit of logarithm of ozone in the top layers against pressure-scaled height to determine power law coefficient σ
9) Adjusts top layers ozone amounts according to the power law.
10) Integrates profile ozone to obtain total ozone.
11) Exits iteration if desired accuracy is met; otherwise repeats above procedures.
12) Calculates ozone layer partial pressure and mixing ratio.
13) Calls INVERSE to calculate the transpose of the Rodgers contribution function $D_n^T = S_{aux}^{-1} * K_{aux}$
14) Calculates absolute averaging kernel $AK = D_n * K_n$
15) Calculates solution covariance $S = S_a - D_n * K_{aux}$

vi. Calls CONVERT20 to convert fine (80)-layer retrieved, a priori, and first guess ozone amounts from Rodgers-type solution into corresponding coarse (20)-layer quantities. Also determines estimated measurement errors in 20-layer ozone and total ozone, 10-channel by 20-layer kernel and 20-layer averaging kernel in its relative (fractional) form.

vii. Calls MIXRATIO to determine ozone mixing ratio and its estimated percentage error at each of prescribed pressure levels.

viii. Calls SET_PROFILE_OUTPUT to load output with retrieved ozone profile data.

MONITORING PROCEDURES

The IDPS/ADL system of log files is used. Log files are written per run to $ADL_HOME/log directory. The level of logging is set at run-time by the xml configuration file.

2.2.2.1 Alphabetical Catalog of V8Pro Subroutines

2.2.2.1.1 Subroutine altitude (altitude.f)

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_v8.

2.2.2.1.2 Subroutine aprsbo (stndprof.f)

Subroutine to read in a priori ozone.

Called by total_v8.

2.2.2.1.3 Subroutine aprsbt (stndprof.f)

Subroutine to read in a priori temperature.

Called by total_v8.

2.2.2.1.4 Subroutine blwcld (blwcld.f)

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

Called by total_v8.

2.2.2.1.5 Subroutine cnstnts (start.f)

Subroutine for initializing various constant parameters used in the retrieval.

Called by start.

Calls coffs.

2.2.2.1.6 coffs (start.f)

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

Called by cnstnts.

2.2.2.1.7 Module constants (constants.f)

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

2.2.2.1.8 Module control (control.f)

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

2.2.2.1.9 Subroutine copy_geoloc_to_output (geo_mod.f)

Subroutine copy_geoloc_to_output is a subroutine to place geolocation data into the output.

Called by scaninv8.

2.2.2.1.10 convert20 (profile_datamod.f)

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

Called by profile_v8.

2.2.2.1.11 Subroutine dn_by_dt (dndt.f)

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.

2.2.2.1.12 Subroutine factor (linsolve.f)

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

Called by update and convert20.

2.2.2.1.13 Module geo_mod (geo_mod.f)

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.

2.2.2.1.14 Subroutine getmsr (getmsr.f)

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_v8.

2.2.2.1.15 Subroutine getrng (getrng.f)

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 reflecv8 and residue.

2.2.2.1.16 Subroutine getshape (getshape.f)

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_v8.

2.2.2.1.17 Subroutine init_dndt (dndt.f)

Subroutine init_dndt.f is a subroutine to initialize ozone absorption coefficients for profile channels.

Called by start.

2.2.2.1.18 Subroutine init_dndt_toz (dndt.f)

Subroutine init_dndt_toz is a subroutine to initialize ozone absorption coefficients for total ozone channels.

Called by start.

2.2.2.1.19 Subroutine init_retrieval (init_retrieval.f)

Subroutine init_retrieval.f is a subroutine that begin the retrieval process.

Called by o3prov8.

Calls read_channel_params and start.

2.2.2.1.20 Subroutine inter (inter.f)

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 scaninv8. Calls insurf and incovr.

2.2.2.1.21 Subroutine interp_dndx (msr.f)

Subroutine interp_dndx is a subroutine to interpolate table entries.

Called by getmsr_single_chan and msr_component.

2.2.2.1.22 Subroutine interp_rad (msr.f)

Subroutine interp_rad is a subroutine to interpolate table entries in pressure.

Called by rad_msr and iztrsb.

Calls interp_sza_vza.

2.2.2.1.23 Subroutine interp_sza_vza (msr.f)

Subroutine interp_sza_vza is a subroutine to interpolate table entries in solar and viewing angles.

Called by interp_rad.

2.2.2.1.24 Subroutine interpol_kern (interpol_kern.f)

Subroutine interpol_kern is a subroutine to interpolate a multiple scattering kernel to a finer pressure level.

Called by profile_v8.

2.2.2.1.25 Subroutine interpol_qo3 (interpol_qo3.f)

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_v8.

2.2.2.1.26 Subroutine interpol_t (interpol_t.f)

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_v8.

2.2.2.1.27 Subroutine inverse (linsolve.f)

Subroutine inverse inverts a matrix.

Called by o3_retrieval, convert20, and update.

2.2.2.1.28 Subroutine iztrsb (iztrsb.f)

Subroutine iztrsb is a subroutine to compute components of the nvalue calculation from radiative transfer tables. It performs interpolations of the table parameters i_0, T_r, and s_b, which are used by the calling 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, reflecv8, and residue.

Calls interp_rad.

2.2.2.1.29 Subroutine linear_fit (linear_fit.f)

Subroutine linear_fit is a subroutine to do a linear least squares fit of a set of points.

Called by o3_retrieval.

2.2.2.1.30 Module lpoly (lpoly.f)

Module lpoly is a module to define lagrangian interpolation coefficients. Used in interp_dndx, interp_sza_vza, , scaninv8, and cnstnts.

2.2.2.1.31 Subroutine mixratio (mixratio.f)

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_v8.

Calls splinev8.

2.2.2.1.32 Module msr (msr.f)

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

2.2.2.1.33 Module msr_temp_adjust (msr.f)

Subroutine msr_temp_adjust is a subroutine to compute adjustments for temperature diffferences.

Calls dn_by_dt.

Called by total_v8.

2.2.2.1.34 Subroutine nvbrac (oznot.f)

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

Called by oznot.

2.2.2.1.35 Subroutine o3_retrieval (o3_retrieval.f)

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_v8.

2.2.2.1.36 Subroutine o3prov8 (o3prov8.f)

Subroutine o3prov8 is a high level subroutine that initializes the retrieval and starts the total ozone computation. If successful it then calls the ozone profile subroutine.

Calls init_retrieval, total_v8 and profile_v8.

Called by pprod_63.f.

2.2.2.1.37 Subroutine o3_snglscatt (o3_snglscatt.f)

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.

2.2.2.1.38 Subroutine oznot (oznot.f)

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

Called by total_v8.

Calls iztrsb, getrngand nvbrac.

2.2.2.1.39 Subroutine ozone_v8 (ozone_v8.f)

Subroutine ozone_v8 is a subroutine to compute step3 ozone or best ozone for the total ozone algorithm.

Called by total_v8.

2.2.2.1.40 Module output (output.f)

Module output is a module that stores values for output.

2.2.2.1.41 Function pintrp (pterp.f)

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

2.2.2.1.42 Subroutine prfind (reflecv8.f)

Subroutine prfind finds table entries for reflectivity computations.

Called by reflecv8.

2.2.2.1.43 Module pterp (pterp.f)

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

2.2.2.1.44 Module press_interp (msr.f)

Function press_interp is a function to interpolate in pressure using lagrangian interpolation.

Called in interp_rad.

2.2.2.1.45 Subroutine profile_v8 (profile.f)

Subroutine profile_v8 is a high level subroutine that does the ozone profile estimation. This is the sub-driver for profile ozone retrieval.

Calls Interpol_qo3, Interpol_t, Interpol_kern, o3_retrieval, set_profile_output, convert20, mixratio, altitude, and splinev8.

Called by o3prov8.

2.2.2.1.46 Module profile_data_module (profile_datamod.f)

Module profile_data_module is a module that stores input data to the ozone profile estimation algorithm.

2.2.2.1.47 Subroutine rad_msr (msr.f)

Subroutine rad_msr is a subroutine to perform N-value table computations.

Calls interp_rad.

Called by total_v8.

2.2.2.1.48 Subroutine rdcons (constants.f)

Subroutine rdcons is in constants.f. 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.

2.2.2.1.49 Subroutine read_clim (stnd_prof.f)

Subroutine read_clim is a subroutine to read in climatological profiles.

Called by start.

2.2.2.1.50 Subroutine read_instrument_table (msr.f)

Subroutine read_instrument table is a subroutine to read in instrument tables.

Called by read_msr_tables.

2.2.2.1.51 Subroutine read_instrument_dndx (msr.f)

Subroutine read_instrument_dndx is a subroutine to read in instrument sensitivity tables.

Called by read_msr_tables.

2.2.2.1.52 Subroutine read_msr_tables (msr.f)

Subroutine read_msr_tables is a subroutine to read in multiple scattering tables.

Called by start.

Calls read_instrument_table and read_instrument_dndx.

2.2.2.1.53 Subroutine reflecv8 (reflecv8.f)

Subroutine reflecv8 is a subroutine to compute reflectivity values using measured nvalue and computed nvalue.

Calls prfind, iztrsb and getrng.

Called by total_v8.

2.2.2.1.54 Subroutine refl_360 (refl_360.f)

Subroutine refl_360 is a subroutine to compute the reflectivity at the longest wavelength measurement.

Calls iztrsb.

Called by total_v8.

2.2.2.1.55 Subroutine resadj (resadj.f)

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

Called by total_v8.

2.2.2.1.56 Subroutine residue (residue.f)

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_v8.

2.2.2.1.57 Subroutine residue_single_chan (residue.f)

Subroutine residue_single_chan is a subroutine to compute residuals for single channels.

Calls iztrsb and getrng.

Called by residue.

2.2.2.1.58 Subroutine scaninv8 (scaninv8.f) see scanin.f

Subroutine scaninv8 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_v8.

2.2.2.1.59 Subroutine set_best_ozone_chans (control.f)

Subroutine to set the ozone channels.

Called by rdcons.

2.2.2.1.60 Subroutine seterr (seterr.f)

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

Called by total_v8.

2.2.2.1.61 Subroutine set_profile_output (profile_v8.f)

Subroutine set_profile_output is a subroutine to load profile ozone variables for a scan.

Calls altitude and spline.

Called by profile_v8.

2.2.2.1.62 Subroutine set_total (total_v8.f)

Subroutine set_total is a subroutine to load total ozone variables for a scan.

Called by total_v8.

2.2.2.1.63 Subroutine splinev8 (splinev8.f)

Subroutine splinev8 is a subroutine to perform clamped cubic spline implementation.

Called by interpol_qo3, interpol_t, mixratio, and profile.

2.2.2.1.64 Subroutine start (start.f)

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.

2.2.2.1.65 Module stndprof (stndprof.f)

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.

2.2.2.1.66 Subroutine stnp81 (stnp81.f)

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_v8.

2.2.2.1.67 Subroutine total_v8 (total.f)

Subroutine total_v8 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_v8, resadj, blwcld, seterr and set_total_output. Called by o3prov8.

2.2.2.1.68 Module totret (totret.f)

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

2.2.2.1.69 Subroutine update (update.f)

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..

2.2.3 Graceful Degradation

2.2.3.1 Graceful Degradation Inputs

No new inputs.

2.2.3.2 Graceful Degradation Processing

No new processing.

2.2.3.3 Graceful Degradation Outputs

No new output.

3.0 GLOSSARY/ACRONYM LIST

3.1 Glossary

Table 14. Glossary

Term	Description
Algorithm	A formula or set of steps for solving a particular problem. Algorithms can be expressed in any language, from natural languages like English to mathematical expressions to programming languages like FORTRAN. On NPOESS, an algorithm consists of: 1. A theoretical description (i.e., science/mathematical basis) 2. A computer implementation description (i.e., method of solution) 3. A computer implementation (i.e., code)
Algorithm Configuration Control Board (ACCB)	Interdisciplinary team of scientific and engineering personnel responsible for the approval and disposition of algorithm acceptance, verification, development and testing transitions. Chaired by the Algorithm Implementation Process Lead, members include representatives from IWPTB, Systems Engineering & Integration IPT, System Test IPT and IDPS IPT.
Algorithm Verification	Algorithm Team science personnel verify science-grade software delivered by an algorithm provider for compliance with data quality and timeliness requirements. This activity is nominally performed at the IWPTB facility. Delivered code is executed on compatible IWPTB computing platforms. Minor hosting modifications may be made to allow code execution. Optionally, verification may be performed at the Algorithm Provider's facility if warranted due to technical, schedule or cost considerations.
EDR Algorithm	Scientific description and corresponding software and test data necessary to produce one or more environmental data records. The scientific computational basis for the production of each data record is described in an ATBD. At a minimum, implemented software is science-grade and includes test data demonstrating data quality compliance.
Environmental Data Record (EDR)	*[IORD Definition]* Data record produced when an algorithm is used to convert Raw Data Records (RDRs) to geophysical parameters (including ancillary parameters, e.g., cloud clear radiation, etc.). *[Supplementary Definition]* An Environmental Data Record (EDR) represents the state of the environment, and the related information needed to access and understand the record. Specifically, it is a set of related data items that describe one or more related estimated environmental parameters over a limited time-space range. The parameters are located by time and Earth coordinates. EDRs may have been resampled if they are created from multiple data sources with different sampling patterns. An EDR is created from one or more NPOESS SDRs or EDRs, plus ancillary environmental data provided by others. EDR metadata contains references to its processing history, spatial and temporal coverage, and quality.
Operational Code	Verified science-grade software, delivered by an algorithm provider and verified by IWPTB, is developed into operational-grade code by the IDPS IPT.
Operational-Grade Software	Code that produces data records compliant with the System Specification requirements for data quality and IDPS timeliness and operational infrastructure. The software is modular relative to the IDPS infrastructure and compliant with IDPS application programming interfaces (APIs) as specified for TDR/SDR or EDR code.

Term	Description
Raw Data Record (RDR)	*[IORD Definition]* Full resolution digital sensor data, time referenced and earth located, with absolute radiometric and geometric calibration coefficients appended, but not applied, to the data. Aggregates (sums or weighted averages) of detector samples are considered to be full resolution data if the aggregation is normally performed to meet resolution and other requirements. Sensor data shall be unprocessed with the following exceptions: time delay and integration (TDI), detector array non-uniformity correction (i.e., offset and responsivity equalization), and data compression are allowed. Lossy data compression is allowed only if the total measurement error is dominated by error sources other than the data compression algorithm. All calibration data will be retained and communicated to the ground without lossy compression. *[Supplementary Definition]* A Raw Data Record (RDR) is a logical grouping of raw data output by a sensor, and related information needed to process the record into an SDR or TDR. Specifically, it is a set of unmodified raw data (mission and housekeeping) produced by a sensor suite, one sensor, or a reasonable subset of a sensor (e.g., channel or channel group), over a specified, limited time range. Along with the sensor data, the RDR includes auxiliary data from other portions of NPOESS (space or ground) needed to recreate the sensor measurement, to correct the measurement for known distortions, and to locate the measurement in time and space, through subsequent processing. Metadata is associated with the sensor and auxiliary data to permit its effective use.
Retrieval Algorithm	A science-based algorithm used to 'retrieve' a set of environmental/geophysical parameters (EDR) from calibrated and geolocated sensor data (SDR). Synonym for EDR processing.
Science Algorithm	The theoretical description and a corresponding software implementation needed to produce an NPP/NPOESS data product (TDR, SDR or EDR). The former is described in an ATBD. The latter is typically developed for a research setting and characterized as "science-grade".
Science Algorithm Provider	Organization responsible for development and/or delivery of TDR/SDR or EDR algorithms associated with a given sensor.
Science-Grade Software	Code that produces data records in accordance with the science algorithm data quality requirements. This code, typically, has no software requirements for implementation language, targeted operating system, modularity, input and output data format or any other design discipline or assumed infrastructure.
SDR/TDR Algorithm	Scientific description and corresponding software and test data necessary to produce a Temperature Data Record and/or Sensor Data Record given a sensor's Raw Data Record. The scientific computational basis for the production of each data record is described in an Algorithm Theoretical Basis Document (ATBD). At a minimum, implemented software is science-grade and includes test data demonstrating data quality compliance.
Sensor Data Record (SDR)	*[IORD Definition]* Data record produced when an algorithm is used to convert Raw Data Records (RDRs) to calibrated brightness temperatures with associated ephemeris data. The existence of the SDRs provides reversible data tracking back from the EDRs to the raw data. *[Supplementary Definition]* A Sensor Data Record (SDR) is the recreated input to a sensor, and the related information needed to access and understand the record. Specifically, it is a set of incident flux estimates made by a sensor, over a limited time interval, with annotations that permit its effective use. The environmental flux estimates at the sensor aperture are corrected for sensor effects. The estimates are reported in physically meaningful units, usually in terms of an angular or spatial and temporal distribution at the sensor location, as a function of spectrum, polarization, or delay, and always at full resolution. When meaningful, the flux is also associated with the point on the Earth geoid from which it apparently originated. Also, when meaningful, the sensor flux is converted to an equivalent top-of-atmosphere (TOA) brightness. The associated metadata includes a record of the processing and sources from which the SDR was created, and other information needed to understand the data.

Term	Description
Model Validation	The process of determining the degree to which a model is an accurate representation of the real-world from the perspective of the intended uses of the model [Ref.: DoDD 5000.59-DoD Modeling and Simulation Management].
Model Verification	The process of determining that a model implementation accurately represents the developer's conceptual description and specifications [Ref.: DoDD 5000.59-DoD Modeling and Simulation Management].

3.2 Acronyms

Table 15. Acronyms

Acronym	Description
ATBD	Algorithm Theoretical Basis Document
CDFCB-X	Common Data Format Control Book - External
CrIS	Cross-Track Infrared Sounder
DMS	Data Management System
DP	Data Product
DPIS	Data Processor Inter-Subsystem
DQN	Data Quality Notification
DQTT	Data Quality Threshold Table
DU	Dobson Unit
EDR	Environmental Data Record
ICD	Interface Control Document
IDPS	Interface Data Processor Segment
INF	Infrastructure
LUT	Look-up Table
NA	Non-Applicable
NASA	National Aeronautics and Space Administration
NOAA	National Oceanic and Atmospheric Administration
NPOESS	National Polar-Orbiting Environmental Satellite System
NP	Nadir Profile
OMPS	Ozone Mapping and Profiling Suite
PMF	Product Master File
RDR	Raw Data Records
SBUV	Solar Backscatter Ultraviolet Spectrometer
Sci2Ops	Science To Operational
SDR	Sensor Data Record
SI	Software Item
TBD	To Be Determined
TBR	To Be Resolved
TC	Total Column
TDR	Temperature Data Record
UTC	Universal Time Coordinated
VIIRS	Visible/Infrared Imager Radiometer Suite

4.0 OPEN ISSUES

Table 16. List of OAD TBD/TBR

No	Description	Resolution Date
None		

5.0 APPENDIX A. FLOW CHARTS FOR V8PRO

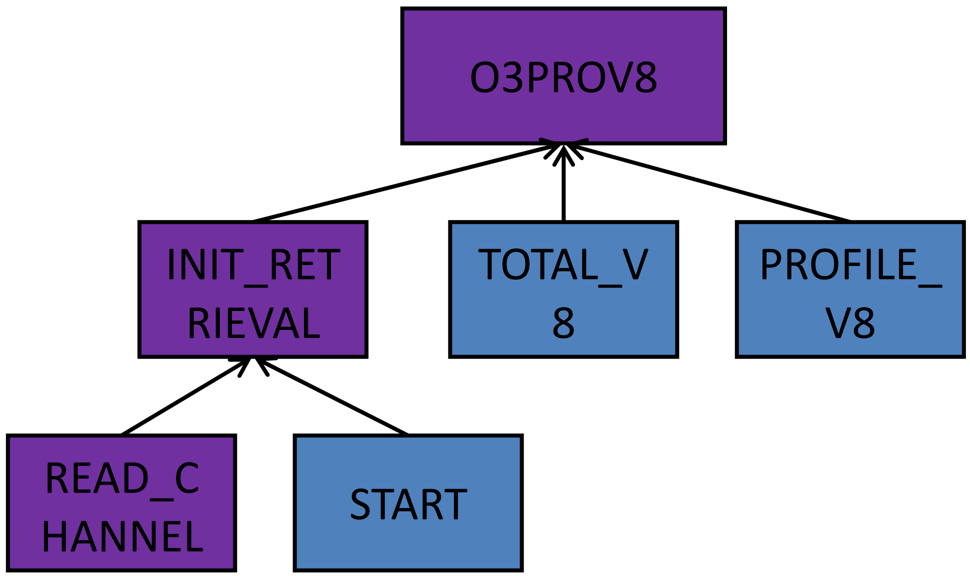

Figure 5. Nadir Top Level Flow Chart for the Version 8 Ozone Profile Retrieval Algorithm

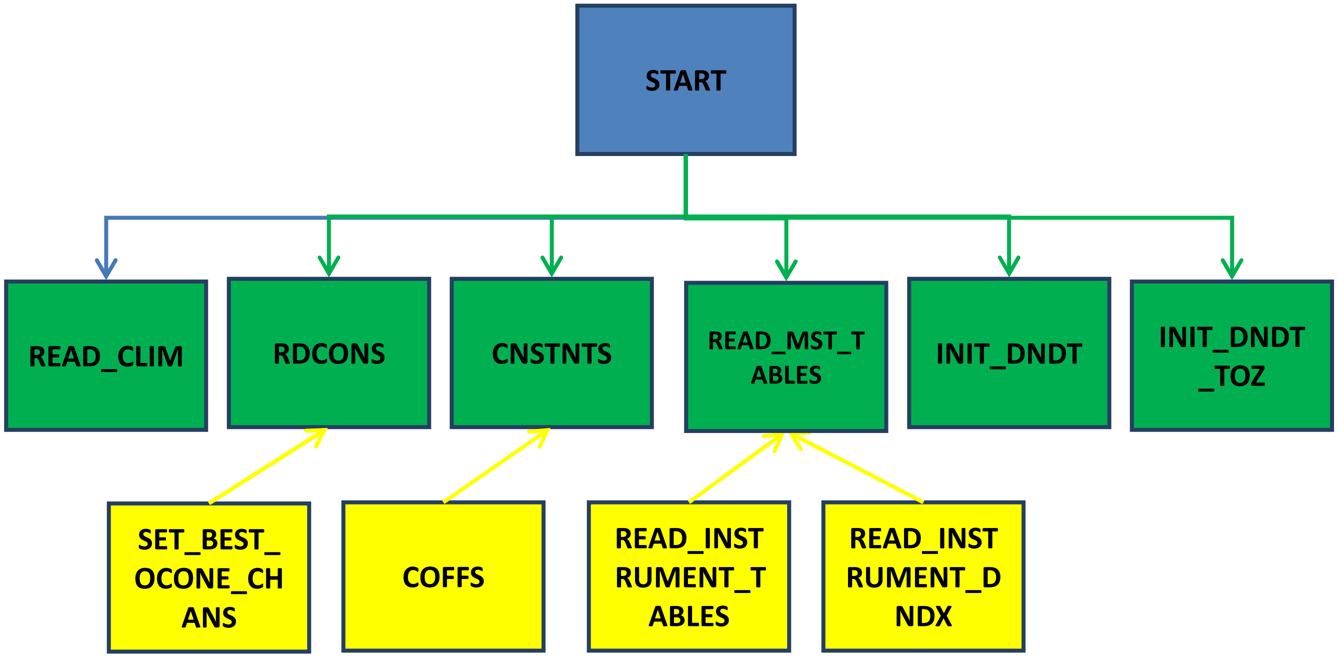

Figure 6. Initialization Flow Chart for the Version 8 Ozone Profile Retrieval Algorithm

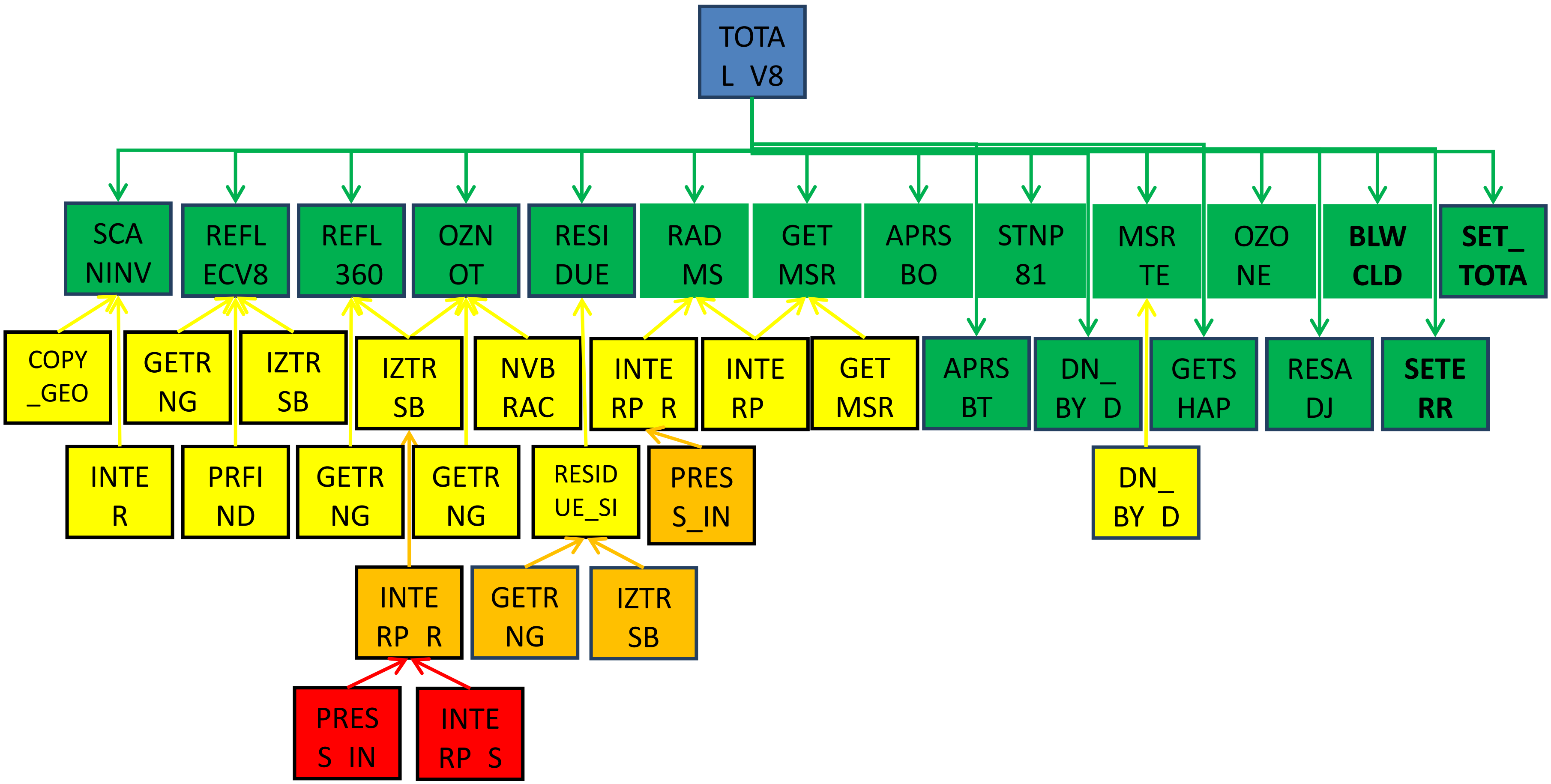

Figure 7. Total Ozone Flow Chart for the Version 8 Ozone Profile Retrieval Algorithm

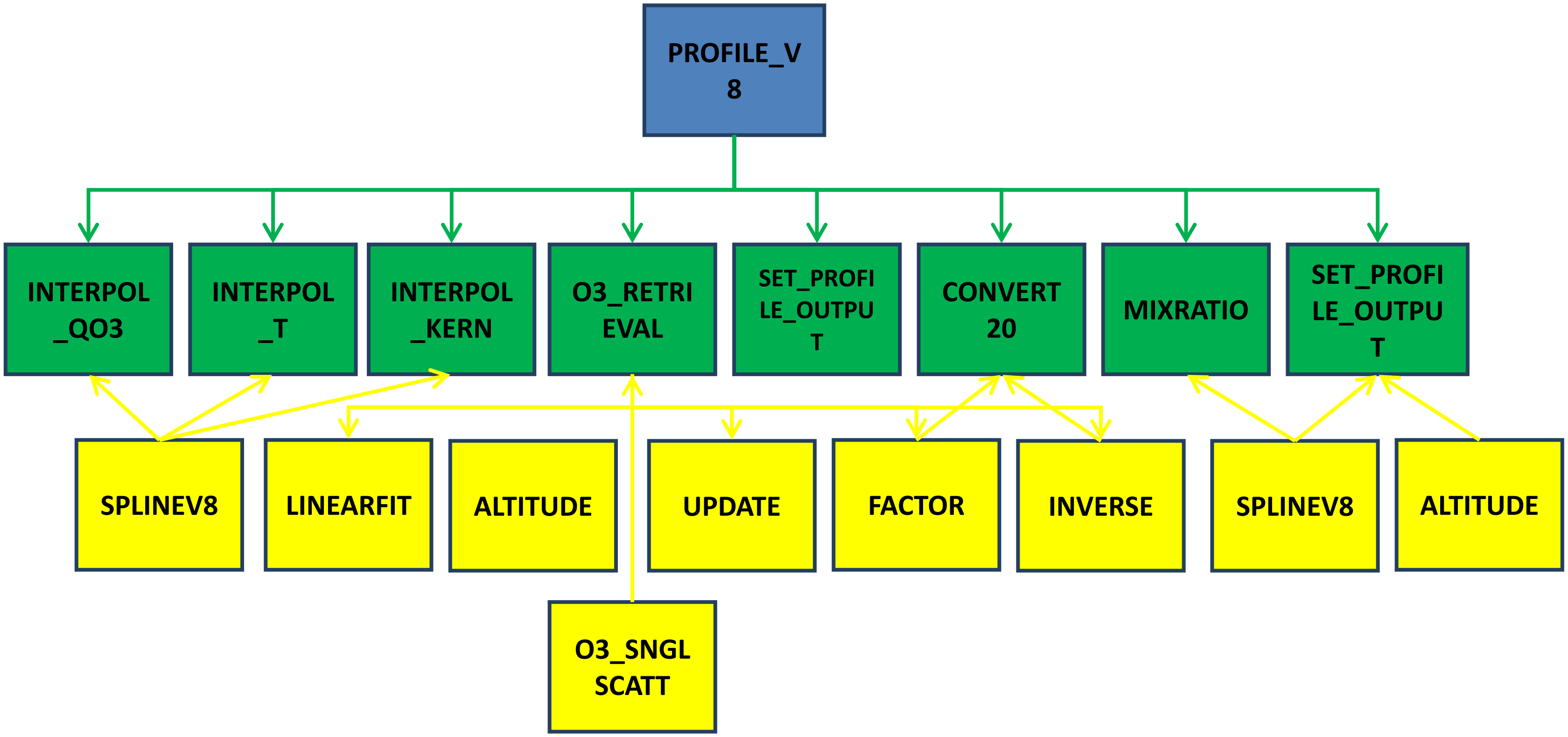

Figure 8. Ozone Profile Flow Chart for the Version 8 Ozone Profile Retrieval Algorithm