Effective Date: January 18, 2012
Revision A

GSFC JPSS CMO
January 25, 2012
Released

Joint Polar Satellite System (JPSS), Ground
Code 474
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 Public Release

The information provided herein does not contain technical data as defined in the International Traffic in Arms Regulations (ITAR) 22 CFC 120.10. This document has been approved For Public Release to the NOAA Comprehensive Large Array-data Stewardship System (CLASS).

Goddard Space Flight Center
Greenbelt, Maryland

National Aeronautics and
Space Administration

This page intentionally left blank.

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

JPSS Electronic Signature Page

Prepared By:

Neal Baker
JPSS Data Products and Algorithms, Senior Engineering Advisor
(Electronic Approvals available online at (https://jpssmis.gsfc.nasa.gov/mainmenu_dsp.cfm)

Approved By:

Heather Kilcoyne
DPA Manager
(Electronic Approvals available online at (https://jpssmis.gsfc.nasa.gov/mainmenu_dsp.cfm)

Goddard Space Flight Center
Greenbelt, Maryland

This page intentionally left blank.

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:

JPSS Configuration Management Office
NASA/GSFC
Code 474
Greenbelt, MD 20771

This page intentionally left blank.

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.

This page intentionally left blank.

Doc No: D38045
Rev C4
Date: 07 Nov 2011
Subcontract No. 7600002744

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)

APPROVAL SIGNATURES:

____

Stephen E. Ellefson Date
ING/PRO Lead

____

Gabriela A. Ostler Date
Mission Assurance and Enterprise Effectiveness (MAEE)

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

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

PREPARED BY:

Scott Farrow *A&DP OMPS Mission & Products Lead*	*Date*	Paul D. Siebels *IDPS PRO SW Manager*	*Date*

ELECTRONIC APPROVAL SIGNATURES:

Roy Tsugawa *SEIT Lead & ACCB Chair*	*Date*	Bob Hughes *Algorithm Implementation Thread Lead*	*Date*
Bob Hughes *Data Product System Engineering Lead*	*Date*	Stephen E. Ellefson *IDPS Processing SI Lead*	*Date*

Prepared by
Northrop Grumman Space Technology
One Space Park
Redondo Beach, CA 90278

Prepared for
Department of the Air Force
NPOESS Integrated Program Office
C/O SMC/CIK
2420 Vela Way, Suite 1467-A8
Los Angeles AFB, CA 90245-4659

Under
Contract No. F04701-02-C-0502

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	

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

Table of Contents

List of Figures

List of Tables

1.0 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 algorithm(s) required to create the Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Intermediate Product (IP).The theoretical basis for this algorithm is described in the OMPS Nadir Profile Ozone Algorithm Theoretical basis Document (ATBD), 474-00026.

1.3 References

1.3.1 Document References

The science and system engineering documents relevant to the algorithms described in this OAD are listed in Table 1.

Table 1: Reference Documents

Document Title	Document Number/Revision	Revision Date
OMPS Nadir Profile Ozone Algorithm Theoretical basis Document (ATBD)	474-00026	22 Apr 2011
NPOESS Calibration and Validation Plan Vol. 5: OMPS	D34484	17 Dec 2002
OMPS Algorithm Test and Verification Plan	D38041	13 Feb2004
OMPS Algorithm Verification Status Report	D36812 Version 1.0	31 Mar 2003
Operational Algorithm Description Document for Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Sensor Data Record (SDR)	474-00081, Rev A	27 Jan 2012
Operational Algorithm Description Document for Ozone Mapping and Profiler Suite (OMPS) Total Column (TC) Sensor	474-00077, Rev A	27 Jan 2012

Document Title	Document Number/Revision	Revision Date
Data Records (SDR)		
JPSS CGS Data Processor Inter-subsystem Interface Control Document (DPIS ICD) Vol I – IV	IC60917-IDP-002, Rev C	29-Sep-11
JPSS Environmental Data Record (EDR) Production Report for NPP	474-00012 Rev. A	09 Feb 2011
JPSS Environmental Data Record (EDR) Interdependency Report (IR) for NPP	474-0007 Rev. A	09 Feb 2011
JPSS Common Data Format Control Book - External - Volume I - Overview	474-00001-01, Rev-	10-Dec-10
JPSS Common Data Format Control Book - External - Volume II - RDR Formats	474-00001-02, Rev-	10-Dec-10
JPSS Common Data Format Control Book - External - Volume III - SDR/TDR Formats	474-00001-03, Rev-	16-Feb-11
JPSS Common Data Format Control Book - External - Volume IV - Part I - IPs, ARPs, and Geolocation Data	474-00001-04-01, Rev-	10-Dec-10
JPSS CDFCB - External - Volume IV - Part II - Imagery, Atmospheric, and Cloud EDRs	474-00001-04-02, Rev-	10-Dec-10
JPSS Common Data Format Control Book - External - Volume IV - Part III - Land and Ocean/Water EDRs	474-00001-04-03, Rev-	10-Dec-10
JPSS Common Data Format Control Book - External - Volume IV - Part IV - Earth Radiation Budget and Space EDRs	474-00001-04-04, Rev-	18-Feb-11
JPSS Common Data Format Control Book - External - Volume V - Metadata	474-00001-05, Rev-	16-Feb-11
JPSS CDFCB - External - Volume VI - Ancillary Data, Auxiliary Data, Messages, and Reports	474-00001-06, Rev-	10-Dec-10
JPSS Common Data Format Control Book - External - Volume VII - Part I - JPSS Downlink Data Formats	474-00001-07-01, Rev-	16-Feb-11
JPSS CDFCB - External - Volume VII - Part 2 - JPSS Downlink Data Formats - CrIS	474-00001-07-02, Rev-	16-Feb-11
JPSS CDFCB - External - Volume VII - Part 3 - JPSS Downlink Data Formats - OMPS	474-00001-07-03, Rev-	16-Feb-11
JPSS CDFCB - External - Volume VII - Part 4 - JPSS Downlink Data Formats - ATMS	474-00001-07-04, Rev-	16-Feb-11
JPSS CDFCB - External - Volume VII - Part 5 - JPSS Downlink Data Formats - VIIRS	474-00001-07-05, Rev-	16-Feb-11
JPSS Common Data Format Control Book - External - Volume VIII - Look Up Table Formats	474-00001-08, Rev-	10-Dec-10
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	21 Jun 2007
JPSS CGS Acronyms and Glossary	LI60917-GND-005, Rev -	17-Oct-11
NPP Mission Data Format Control Book and App A (MDFCB)	472-REF-00057	06 Jan 2011
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

The science and operational code and associated documentation relevant to the algorithms described in this OAD are listed in Table 2.

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
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	Maintaince 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

2.0 ALGORITHM OVERVIEW

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

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 illustrated in Figure 1.

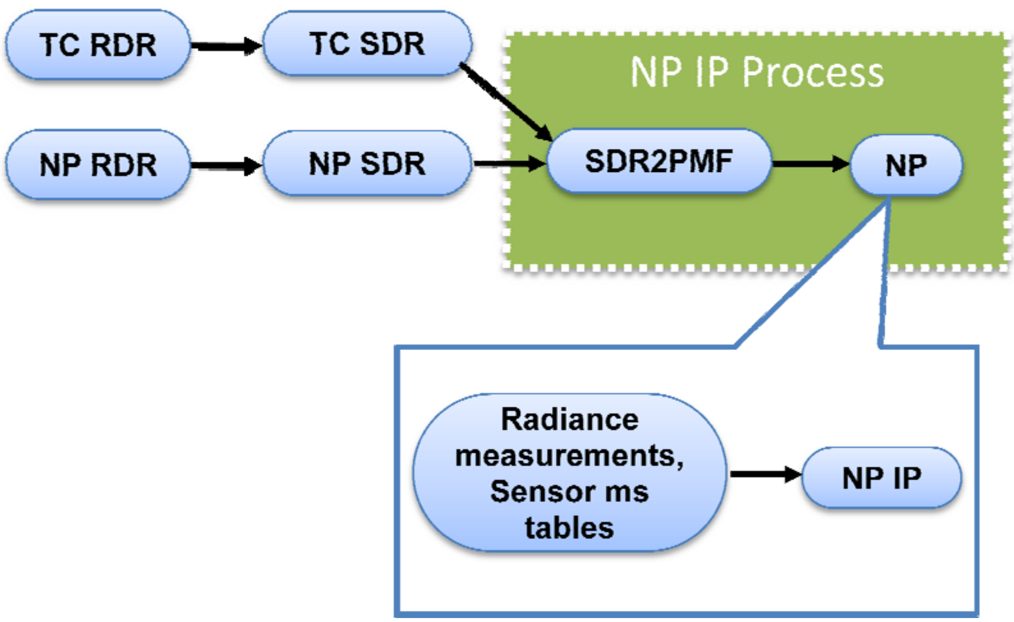

Figure 1: Processing Chain Associated with the OMPS NP Ozone Algorithm

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 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 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.

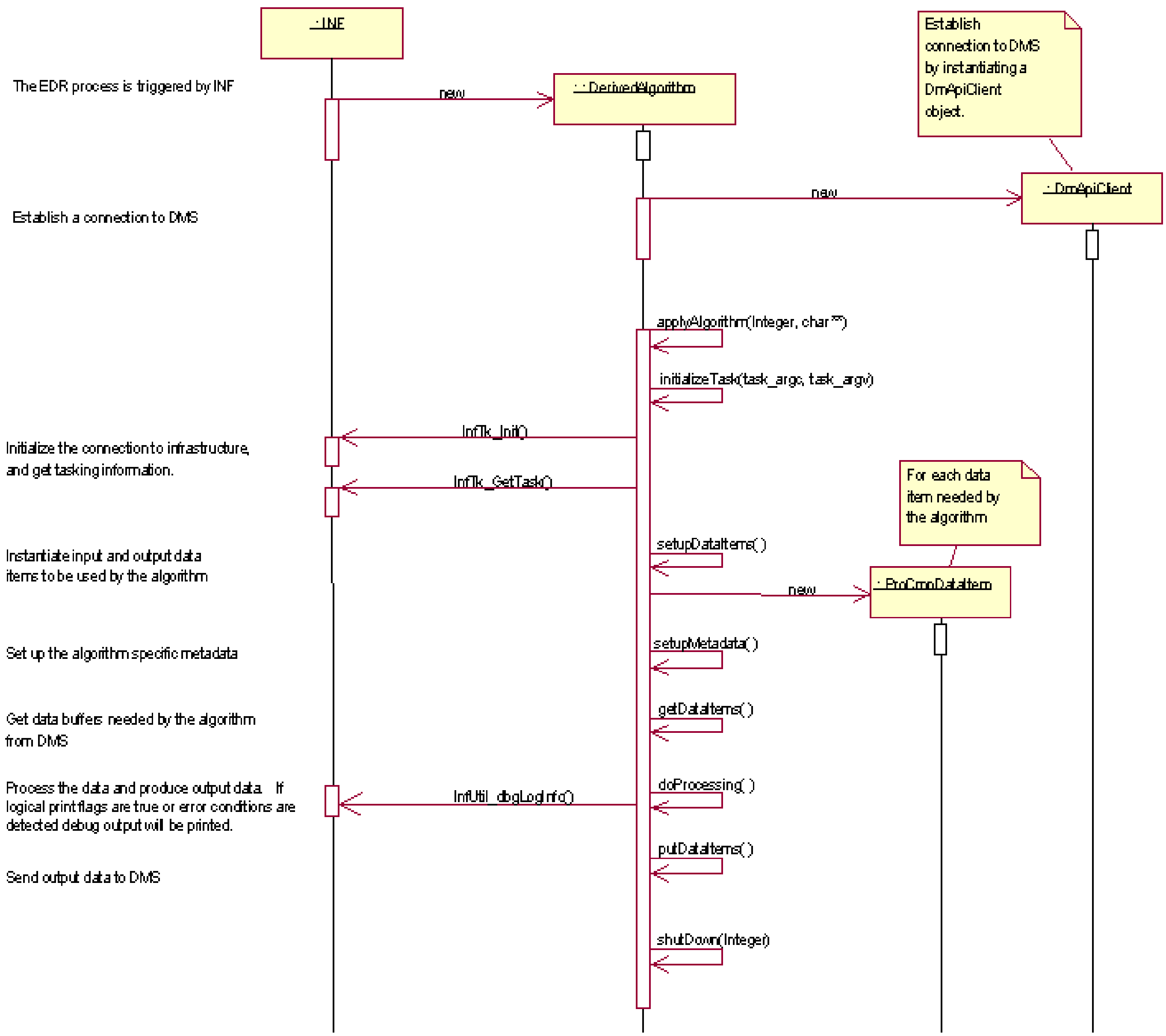

Figure 2: IPO Model Interface to INF and DMS

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, D34862, 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	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	8	Real*4	Latitude (for SBUV/2 was average latitude for total ozone wavelengths)	Input SDR file	Degrees
LONTOZ	9	Real*4	Longitude (for SBUV/2 was average longitude for total ozone wavelengths)	Input SDR file	Degrees
SZATOZ	10	Real*4	Solar Zenith Angle (for SBUV/2 was average solar zenith angle for total ozone wavelengths)	Input SDR file	Degrees
NPHOTTOZ	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	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

Input	Word	Type	Description	Original Source	Units
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
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
FRSTGUESST OZ	81	Real*4	Total ozone for first guess	Output from SBUV/2 retrieval algorithm	DU

Input	Word	Type	Description	Original Source	Units
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
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

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

Input	Word	Type	Description	Original Source	Units
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

2.1.1.1.1 Look-Up Tables

The SBUV/2 processor utilizes look-up tables. The LUT contains values for both the profile and total ozone calculations contained in the SBUV/2 processor. Contents of the LUT are described in Table 4.

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

The Nadir Profile algorithm produces two Intermediate Products as shown in Table 5 and Table 6. Refer to the CDFBC-X, D34862, 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	ErrorFlag	Float32 * 1 * 1	See Table 8	Unitless / 0.0 – 20.0
tableIndex	tableIndex	Float32 * 1 * 1	Table selection scheme index	Unitless / Minfloat – Maxfloat

Output	CDFCB-X Name	Type	Description	Units/Valid Range
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
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	TotalO3ErrorCode	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

Output	CDFCB-X Name	Type	Description	Units/Valid Range
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
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.

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.

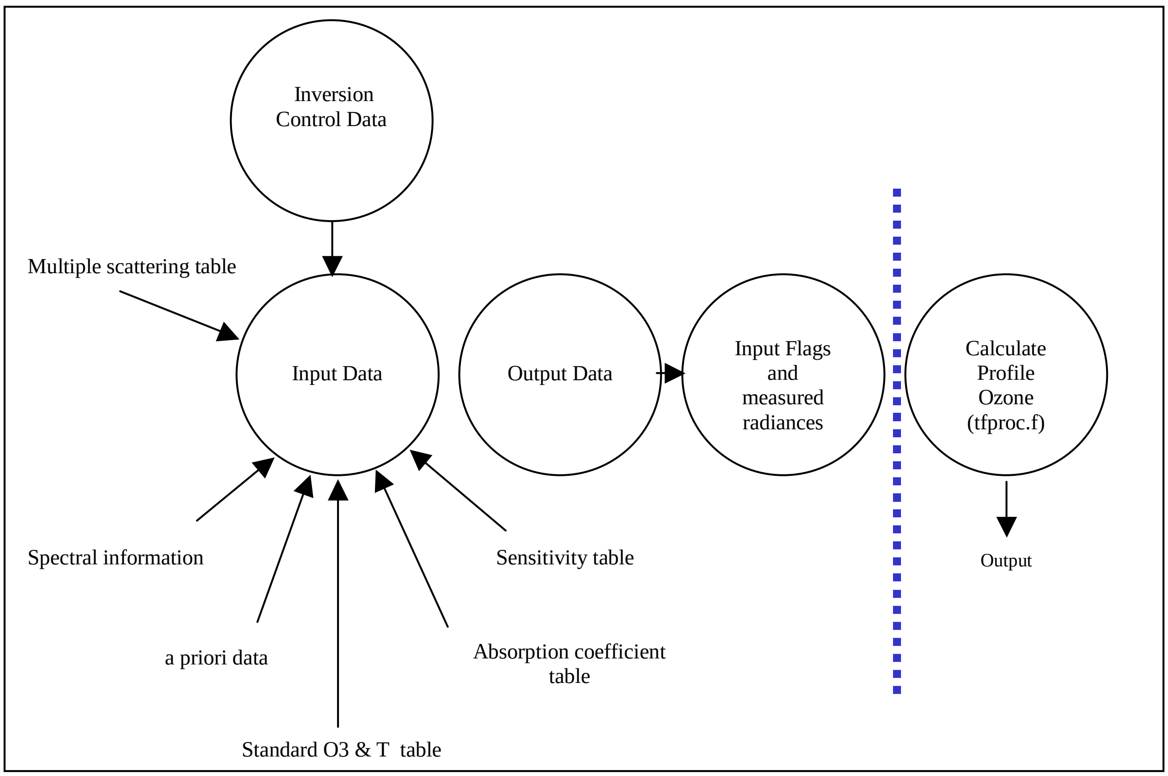

Figure 3: Flow Diagram for the Top-Level Driver pprod_62.f

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 $P_{Effective} = (1-w)P_{cloud} + wP_{terrain}$, 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 = 1	OZONIN = 260
45°< |lat| <= 75°	ILAT = 2	OZONIN = 340
|lat| > 75°	ILAT = 3	OZONIN = 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 $60º \leq \theta_0 \leq 80º$.

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; it's 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.

2.1.2.4.3.10 Subroutine 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.

2.1.2.4.3.11 Subroutine linfit (linfit.f)

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

2.1.2.4.3.12 Subroutine alogam (alogam.f)

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

2.1.2.4.3.13 Subroutine 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

2.1.2.4.3.14 Subroutine stnprf (stnprf.f)

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

2.1.2.4.3.15 Subroutine 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.

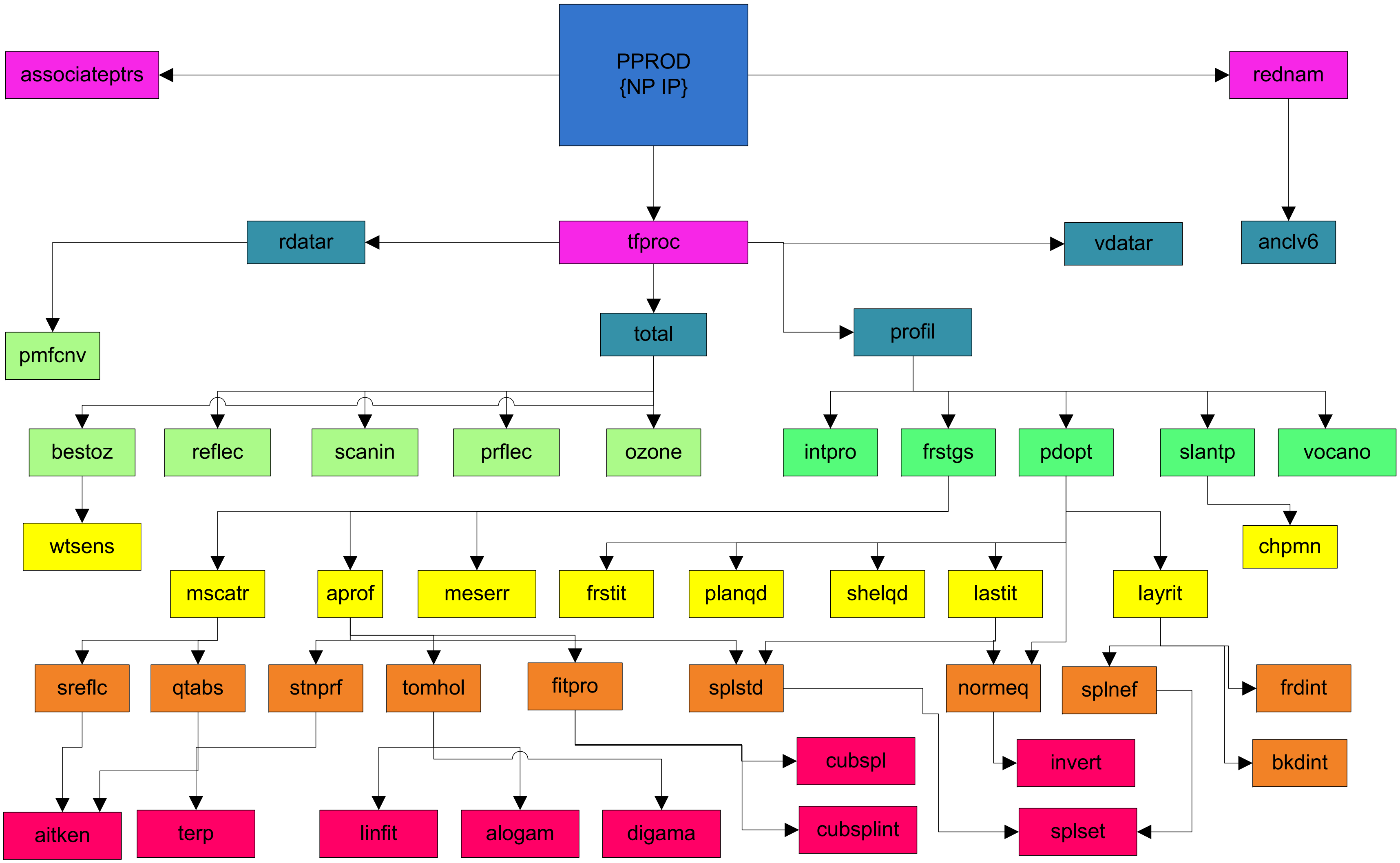

Figure 4: Nadir Profile Flow Diagram

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.

The consistency between best ozone and the A, B or C pair is then checked; the pair used in the comparison is the one with the largest weighting factor (see the NP ATBD for details). The quality flag is set to 4 is inconsistency exists, and best ozone is set to –999. Data that pass flag 4 are assigned a flag value of 0, 1 or 2 as determined by the ozone path (see Table 7):

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.

Values for the total ozone quality flag (CDFCB name is ErrorFlag from Table 5/CDFCB) are summarized below (see Table 8) :

Table 8: Total Ozone Error Code and 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).

Values for the profile quality flag (CDFCB name is TotalO3ErrorCode from Table 5/CDFCB) are summarized below (See Table 9):

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)
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

3.0 GLOSSARY/ACRONYM LIST

3.1 Glossary

Table 10: 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.
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 11: 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 12: List of OAD TBD/TBR

No	Description	Resolution Date
None		