

GSFC JPSS CMO  
May 19, 2015  
Released

**Joint Polar Satellite System (JPSS) Ground Project  
Code 474  
474-00066**

**Joint Polar Satellite System (JPSS)  
Operational Algorithm Description  
(OAD)  
Document for Ozone Mapping and  
Profiler Suite (OMPS) Total Column  
(TC) Environmental Data Records  
(EDR) 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**

**Joint Polar Satellite System (JPSS)  
Operational Algorithm Description (OAD) Document for  
Ozone Mapping and Profiler Suite (OMPS) Total Column  
(TC) Environmental Data Records (EDR) Software  
JPSS Electronic Signature Page**

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**Goddard Space Flight Center  
Greenbelt, Maryland**

## 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 <b>474-CCR-11-0084</b> which converts Operational Algorithm Description Document For for OMPS Total Column (TC) EDR, Rev B of D37031 to a JPSS document, Rev -. This was approved by the JPSS Ground Algorithm ERB on June 3, 2011.
Revision A	01/18/2012	<b>474-CCR-11-0258:</b> This version baselines 474-00066, Joint Polar Satellite System (JPSS) Operational Algorithm Description (OAD) Document for Ozone Mapping and Profiler Suite (OMPS) Total Column (TC) Environmental Data Records (EDR) Software, for the Mx 6 IDPS release. This CCR was approved by the JPSS Algorithm ERB on January 18, 2012.
Revision B	10/09/2012	<b>474-CCR-11-0627:</b> This version authorizes 474-00066, Joint Polar Satellite System (JPSS) Operational Algorithm Description (OAD) Document for Ozone Mapping and Profiler Suite (OMPS) Total Column (TC) Environmental Data Records (EDR) Software, for the Mx 6.1 – 6.3 IDPS releases. Includes <b>ECR-ALG-0035</b> which contains Raytheon PCR031213, OAD: Implement 474-CCR-12-0419 (OMPS TC IP and EDR Modification to Cloud Fraction Calculation) (ADR 4266) updated in section 2.1.2.7. Raytheon PCR031525, OAD: Implement 474-CCR-12-0481 TC IP_EDR Earth Sun Distance (DR 4798) updated mainly on pages 5, 9-10 & 14.
Revision C	05/14/2013	<b>474-CCR-13-0948:</b> This version authorizes 474-00066, JPSS OAD Document for OMPS TC EDR Software, for the Mx 7.0 IDPS release. Includes <b>ECR-ALG-0037</b> which contains Raytheon PCR033339; OAD: PRO: Implement 474-CCR-12-0736 (Modify OMPS TC EDR to Use UV Cloud Top Pressure) (ADR 4955), in Table 4 and sections 2.1.2 & 2.1.3.1. Includes Raytheon PCR032720; CCR-474-13-0916/ECR-ALG-0037: Update applicable OAD filenames/template/Rev/etc. for Mx7 Release.
Revision D	07/10/2013	<b>474-CCR-13-1101:</b> This version authorizes 474-00066, JPSS OAD Document for OMPS TC EDR Software, for the Mx 7.1 IDPS release. Includes Raytheon ECR-ALG-0039/PCR034049: OAD: Implement 474-CCR-13-0893 (TC Ascending/Descending Flag is in Error) (ADR 4804), in section 2.1.4.2.
Revision E	03/05/2014	<b>474-CCR-14-1590:</b> This version authorizes 474-00066, JPSS OAD Document for OMPS TC EDR Software, for the Mx 8.3 IDPS release. Includes Raytheon PCR036543;

		CHILD: PRO: OAD: 474-CCR-13-1215: Profile Mixing Fraction Adjustment - OMPS TC EDR - DR 7310), in section 2.1.2.11 and Table 7.
Revision F	01/07/2015	<b>474-CCR-14-2212:</b> This version authorizes 474-00066, JPSS OAD Document for OMPS TC EDR Software, for the Mx 8.8 IDPS release. Includes Raytheon PCR043877, Child: PRO: 474-CCR-14-2175-Record, OAD: 474-00066_OAD-OMPS-TC-EDR Turn off graceful degradation in OMPS TC EDR when CrIMSS is missing -- DR7817, in Section 2.1.3.1. and updates Tables 7 & 11.
Revision G	05/13/2015	<b>474-CCR-15-2428:</b> This version authorizes 474-00066, JPSS OAD Document for OMPS TC EDR Software, for the Mx 8.9 IDPS release. Includes Raytheon PCR046133, PRO: OAD: 474-CCR-15-2264: Resolve TBDS in 474-00066 OAD For OMPS Total Column EDR Software; in Tables 1, 7 and 11.



**NATIONAL POLAR-ORBITING  
OPERATIONAL ENVIRONMENTAL  
SATELLITE SYSTEM (NPOESS)**

**OPERATIONAL ALGORITHM DESCRIPTION  
DOCUMENT FOR OMPS TOTAL COLUMN  
(TC) EDR**

**SDRL 141  
SYSTEM SPECIFICATION SS22-0096**

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

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

**CAGE NO. 11982**

**Operational Algorithm Description  
For OMPS TC EDR**

**Document Date: Nov 05, 2011**

**Document Number: D37031  
Revision: C5**

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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		 	
Revision/Change Record			Document Number D37031
Revision	Document Date	Revision/Change Description	Pages Affected
---	12-15-03	Initial Release	All
---	3-15-05	Reflects Science To Operational Code Conversion	All
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. 622-1, 304, 305, 624	Title pages & pg 1-2
B2	1-21-10	Updated from TM 2009.510.0058-Rev-A	All
B2	3-30-10	Ensured important details about TC Glueware from NP-EMD.2005.510.0124 were included	Table 3
B3	4-22-10	SDRL Delivery (Includes OAD PR comments)	All
B4	8-13-10	Implemented Tech Memo 2010.510.0028-Rev-B	Tables 1 & 2
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	11-11-10	Updated to implement Tech Memos 2010.510.0072 and 2010.510.0073.	All
C3	12-20-10	Updated for PCR23368	All
C4	09-29-11	Updated for PCR 027828	All
C5	11-05-211	OAD Update for ECR-ALG-0014 (PCR026607)	All

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## 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 algorithms required to create the Ozone Mapping and Profiler Suite (OMPS) Total Column (TC) Environmental Data Record (EDR) and the First Guess Intermediate Product (IP). The theoretical basis for this algorithm is described in the OMPS NADIR Total Column Ozone Algorithm Theoretical Basis Document ATBD, 474-00029.

### 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 Total Column Ozone Algorithm Theoretical Basis Document ATBD	474-00029	Latest
OMPS Nadir Profile Ozone Algorithm Theoretical basis Document (ATBD)	474-00026	Latest
OMPS Command and Telemetry Handbook	V6.6	12 Oct 2004

Document Title	Document Number/Revision	Revision Date
NPP Mission Data Format Control Book and App A (MDFCB)	429-05-02-42-02_MDFCB	Latest
Operational Algorithm Description Document for Ozone Mapping and Profiler Suite (OMPS) Nadir Profile (NP) Sensor Data Record (SDR)	474-00081	Latest
OMPS Algorithm Verification Status Report	D36812 Version 1.0	31 Mar 2003
JPSS CGS Data Processor Inter-subsystem Interface Control Document (DPIS ICD) Vol I – IV	IC60917-IDP-002	Latest
JPSS Environmental Data Record (EDR) Production Report (PR) 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 1.2.3 (All Volumes)	474-00001-01-B0123 CDFCB-X Vol I 474-00001-02-B0123 CDFCB-X Vol II 474-00001-03-B0123 CDFCB-X Vol III 474-00001-04-01-B0123 CDFCB-X Vol IV Part 1 474-00001-04-02-B0123 CDFCB-X Vol IV Part 2 474-00001-04-03-B0123 CDFCB-X Vol IV Part 3 474-00001-04-04-B0123 CDFCB-X Vol IV Part 4 474-00001-05-B0123 CDFCB-X Vol V 474-00001-06-B0123 CDFCB-X Vol VI CDFCB-X Vol VII Part 5 474-00001-08-B0123 CDFCB-X Vol VIII	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

Document Title	Document Number/Revision	Revision Date
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
Joint Polar Satellite System (JPSS) Program Lexicon	470-00041	Latest
NGAS Tech Memo OMPS_TC_EDR_OAD_Updates_Delivery5_1	2009.510.0058 Rev. A	30 Nov 2009
NGAS Tech Memo OMPS TC EDR Cloud Pressure	2010.510.0028-Rev-B	21 Jul 2010
NGAS Tech Memo OMPS_TC_EDR_Reflectivity_Calculations	NP-EMD.2010.510.0072.Rev-A	15 Sep 2010
NGAS Tech Memo OMPS_TC_EDR_Output_Format_Update_and_Var_Init	NP-EMD.2010.510.0073	15 Sep 2010
Joint Polar Satellite System (JPSS) Common Ground System (CGS) IDPS PRO Software User's Manual Part 2	UG60917-IDP-026	Latest
NGAS Tech Memo OMPS TC EDR Fix Zeros in Output	NP-EMD.2011.510.0010	22 Feb 2011
NGAS Tech Memo OMPS TC EDR Output Format Update and Variable Initialization	NP-EMD.2010.510.0073.Rev-A	22 Feb 2011

### 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**

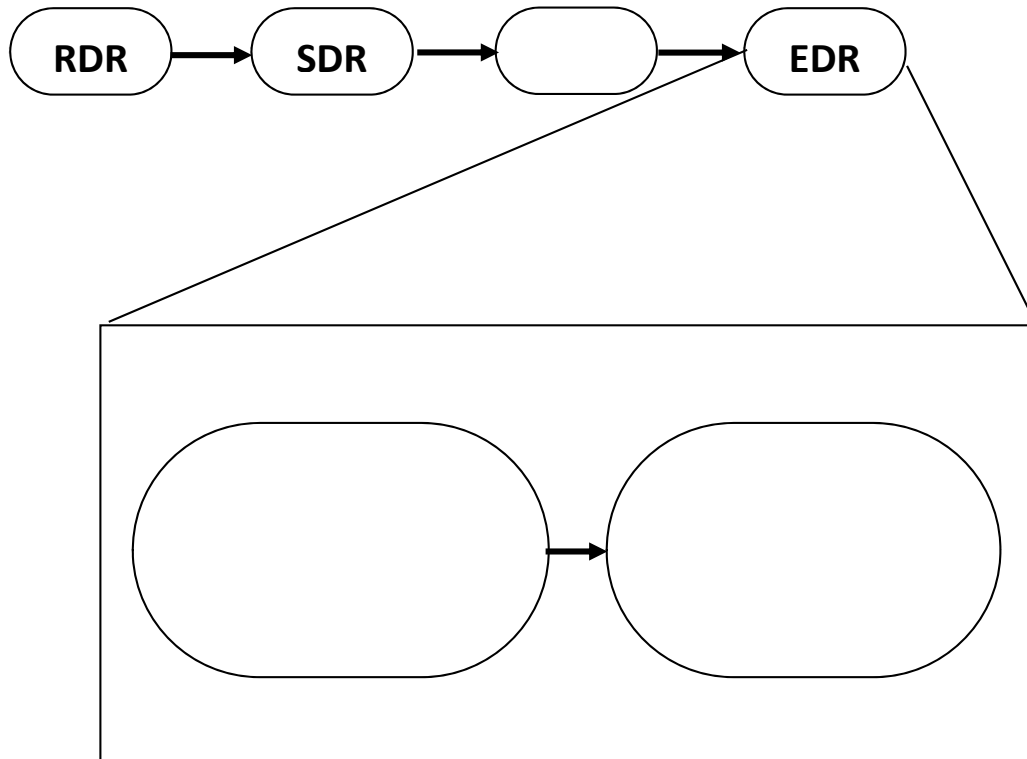
Reference Title	Reference Tag/Revision	Revision Date
OMPS Science Algorithms Delivery	ISTN_OMPS_TC_NGST_2.1	22 Dec 2003
OMPS TC EDR Operational software	Build 1.3. (OAD Rev ---)	23 Apr 2004
OMPS Science Algorithms Delivery	ISTN_OMPS_TC_NGST_2.1.1	01 Apr 2005
OMPS TC EDR Test Plan DPSE Technical Memo	NP-EMD.2005.510.0045	06 Apr 2005
OMPS TC EDR Operational software	Build 1.3. (OAD Rev ---)	25 Feb 2005
OMPS Science Algorithms Delivery	ISTN_OMPS_TC_EDR_NGST_5.1 (OAD: TM 2009.510.0058)	30 Nov 2009
OMPS TC EDR Operational software	Build Maintenance A 2 (MaintA-2) (OAD Rev B2)	23 Mar 2010
SDRL	(OAD Rev B3)	22 Apr 2010
NGAS Tech Memo OMPS TC EDR Cloud Pressure TM 2010.510.0028-Rev-B (PCR024312)	Build Sensor Characterization SC-13 (OAD Rev B4)	13 Aug 2010
ACCB (no code updates)	OAD Rev B	18 Aug 2010
Convergence Update (No code update)	(OAD Rev C1)	20 Oct 2010
Implemented TMs 2010.510.0072,Rev-A & 2010.510.0073 (PCR024770)	Mx.1.5.4.00 (OAD Rev C2)	11 Nov 2010
PCR023368	(OAD Rev C3)	20 Dec 2010

Reference Title	Reference Tag/Revision	Revision Date
PCR027828 (OAD update for ADL)	(OAD Rev C4)	29 Sep 2011
PCR026607 (ECR-ALG-0014 which includes TMs NP-EMD-2010.510.0073.Rev-A and NP-EMD-2011.510.0010) (x-ref PCR026606)	Mx.1.5.6-J (OAD Rev C5)	05 Nov 2011
OAD transitioned to JPSS Program – this table is no longer updated.		



## 2.0 OPERATIONAL ALGORITHM DESCRIPTION

The OMPS TC ozone algorithm is based on the Total Ozone Mapping Spectrometer (TOMS) Version 7 algorithm. This algorithm is similar in concept to previous versions of the algorithm, but contains a number of enhancements that improve the treatment of surface reflectivity, clouds, profile mixing, and high solar zenith angles. The OMPS total ozone EDR is computed after the Sensor Data Record (SDR) and Intermediate Product process is done. This processing relationship is illustrated in Figure 1 below.



**Figure 1: Processing Chain Associated with the OMPS TC Ozone EDR**

The OMPS total ozone EDR benefits from true multi-spectral capability and significant compatibility with the heritage TOMS sensor and algorithm. The OMPS Charge Coupled Device (CCD) combined with the push broom sensor design allows simultaneous measurement of all 35 fields of regard (FOR) across the swath.

### 2.1 OMPS Total Column Ozone EDR Description

#### 2.1.1 Interfaces

The OMPS Total Column (TC) EDR algorithm is initiated by the Infrastructure (INF) Software Item (SI) to begin processing data. INF SI provides tasking information to the algorithm indicating which granule to process. DMS SI provides data storage and retrieval capability. A library of C++ classes is used to implement the SI interfaces. More information regarding these topics is found in document UG60917-IDP-026 with reference in particular to sections regarding

PRO Common (CMN) processing and the IPO Model. The science code ingests all required data in the calcOTC program.

### 2.1.1.1 Inputs

All inputs are ingested in the glueware module, bundled, and passed on to the Main Science Module - calcOTC.f program. Refer to the CDFCB-X, 474-00001 for a detailed description of these inputs. Table 3 below gives IP/EDR Inputs. The TC IP uses climatology for temperature and cloud information and the VIIRS snow/ice gridded IP for snow/ice information. The TC EDR uses CrIMSS and VIIRS products to get temperature, cloud, and snow/ice information. IDPS implemented the SDR2EDR Glueware as a conversion method that is used before calling the calcOTC science algorithm. Data values from the Total Column SDR, Geolocation, and granulated ancillary products are massaged into the format shown in Table 3. Table 4 specifies data from other NPP sensors required by the TC EDR ozone algorithm. Table 5 specifies climatological data required by the TC ozone algorithm (note: some of the databases are only used if external NPP EDRs are not available).

**Table 3. TC EDR Bundled Input**

Input	Type	Description	Units/Valid Range
Pixel-Level Data Items			
Id	character	SDR ID number – unused internally	Unitless
satza	real	Satellite zenith angle	Degrees
sza	real	Solar zenith angle	Degrees
xphi	real	Relative azimuth angle between sensor and solar azimuth angles	Degrees
month	integer	Month of measurement	Month / 1 - 12
xlat	real	Latitude of measurement	Degrees / -90 - 90
xlong	real	Longitude of measurement	Degrees / -180 - 180
prtrop	real	Tropopause pressure	Atmosphere (atm) / 0 - 1.1
xnvalm	real	Log of the normalized radiances for 22 sensor wavelengths	Unitless / 0 - 500
sflux	real	Solar flux for 22 sensor wavelengths	W/m <sup>2</sup> -nm / 0 – 3x10 <sup>7</sup>
sdev	real	Standard deviation representing variability or tropospheric ozone amounts	DU / Real Value
wlenth	real	22 sensor wavelengths for measurement	nm / 290 - 390
tozclim	real	Tropospheric ozone values from climatology at xlat, xlong (4 values for first 4 Umkehr layers) – disabled in indefinite absence of a Limb Profile	Dobson Unit (DU) / 0 - 200
vcf	real	VIIRS cloud fraction	Fraction / 0 – 1.0
pcloud	real	cloud pressure	hPa / 0 – 1013.25
pteran	real	terrain pressure	hPa / 0 – 1013.25
prftemp	real	CrIMSS temperature profile for 11 Umkehr layers	Degrees Kelvin (K) / 170 – 350
presprf	real	CrIMSS pressure profile for 11 Umkehr layers - deprecated	hPa / N/A
isnow	integer	Snow/ice flag	Unitless / 0 - 1

Input	Type	Description	Units/Valid Range
prfoz	real	TOMS V8 Climatology Data	DU / 0 – 999 (0 – 200 for non-fill)
cwavl	real	Wavelength for absorption coefficient	nm / 290 - 390
c0	real	Absorption coefficient at cwavl at 273 K	atm / cm / 0 - 5
c1	real	Linear temperature correction Coefficient to c0	atm / cm / K / 0 - 0.08
c2	real	Quadratic temperature correction Coefficient to c0	atm / cm / K <sup>2</sup> / -0.002 to 0.002
o3abs	real	Ozone absorption coefficients used in SOI algorithm	atm / cm /
so2abs	real	SO <sub>2</sub> absorption coefficients used in SOI algorithm	atm / cm /
so2wav	real	Wavelengths to use in SOI algorithm	nm / 316 – 337
tpflag	integer	Flag controlling use of temperature profile correction	Unitless / 0 or 1
xpflag	integer	Flag controlling use of ozone profile correction	Unitless / 0 or 1
tropflag	integer	Flag controlling use of tropospheric ozone correction	Unitless / 0 or 1
logi0n, z1i0n, z2i0n, ti0n, sbn	real	OMPS northern hemisphere LUT values	See Table 5 / -5 - 100
logi0s, z1i0s, z2i0s, ti0s, sbs	real	OMPS southern hemisphere LUT values	See Table 5 / -5 - 100
dndxlogi0, dndxz1i0, dndxz2i0, dndxti0, dndxsb	real	OMPS sensitivity LUT values	See Table 6 / -5 - 100

**Table 4. Other NPP Products Used by the Total Column IP/EDR Algorithm**

Sensor	Data	Form	Use
CrIMSS	Temperature profile IP	Co-located in 11 Umkehr layers Kelvin	Temperature profile shape (EDR only)
VIIRS	Cloud Top Pressure	Co-located and regridded percent of OMPS footprint covered. Specifically, this is the Cloud Top Parameters IP which is not parallax-corrected.	Input – Not used, overwritten by UV climatology for Cloud top pressure)
VIIRS	Snow Cover EDR	Combined with IST to form fraction snow/ice in FOV	Snow/ice indication over land Calc of normalized radiances (EDR only)
VIIRS	Ice Surface Temperature	Combined with Snow to form fraction snow/ice in FOV	Ice presence over Ocean (EDR only)
VIIRS	Snow/Ice GIP	Fraction snow/ice in FOV	Snow/ice indication over land Calc of normalized radiances (IP Primary, Fallback (GD) for EDR)

**Table 5. Climatological Data Needed by the Total Column Algorithm**

Data	Form	Source	Use
Surface pressure*	0.5° x 0.5° grid In mbars	TUG87 geophysical model (see Weiser, 1987)	Calculation of normalized radiances (IP Primary, GD for EDR)
Cloud pressure*	1° x 1° x 12 month In mbars	ISCCP	Partial cloud algorithm Calculation of normalized radiances (IP Primary, GD for EDR)
Surface reflectivity	1° x 1° x 12 months	Herman and Celarier, JGR, 1997	Calculate radiances
Temperature Profile	1 long zone x 18 lat zones x 11 Umkehr layers x 12 months	TOMS V8	Coverage for hybrid temperature profile where CrIMSS and NCEP data are unavailable – typically for upper 5 Umkehr layers outside of CrIMSS swath.

\* Used if external EDR not available

**2.1.1.1.1 Look-Up Table**

Table 6 displays the contents of the OMPS TC IP/EDR LUT.

**Table 6. OMPS TC IP/EDR LUT Contents**

Parameter	Dimension	Type	Units
logi0n	(274560,7)	Float 32	Unitless
z2i0n	(274560,7)	Float 32	Unitless
sbn	(2288,7)	Float 32	Unitless
Logi0s	(274560,7)	Float 32	Unitless
z2i0s	(274560, 7)	Float 32	Unitless
ti0s	(274560, 7)	Float 32	Unitless
sbs	(274560, 7)	Float 32	Unitless
dndxlogi0	(3294720)	Float 32	Unitless
dndxzli0	(3294720)	Float 32	Unitless
dnxdz2i0	(3294720)	Float 32	Unitless
dndxti0	(3294720)	Float 32	Unitless
dndxsb	(27456)	Float 32	Unitless
cwavl	(22, 7)	Float 32	nm
c0	(22, 7)	Float 32	Atm/cm
c1	(22, 7)	Float 32	Atm/cm/k
c2	(22, 7)	Float 32	Atm/cm/k
stprf	(2, 26, 12)	Float 32	DU
V8OZ	(11, 10, 18, 12)	Float 32	DU
So2o3	(3)	Float 32	DU

**2.1.1.2 Outputs**

The OMPS TC IP and EDR are listed in Table 7.

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

**Table 7. Total Column Ozone Output File Content**

Output	Type	Dimension	Description	Units/Valid Range
columnAmountOz	Float32	5x35	Total Column Ozone	DU/ 50-650
reflectivity	Float32	5x35	Reflectance	Unitless/ -5-120
nValueMeasured	Float32	5x35x22		Unitless/ 0-500
ozoneBelowCloud	Float32	5x35	Ozone below cloud	DU/ 0-200
terrainPressure	Float32	5x35	Surface Pressure	Atm/0-1.1
cloudTopPressure	Float32	5x35	Cloud Top Pressure	Atm/0-1.1
cloudFraction	Float32	5x35	Cloud Fraction	Unitless/0-1
mixingFraction	Float32	5x35	Snow/Ice Fraction	Unitless/- .5-1.5
aerosolIndex	Float32	5x35	Aerosol Index	Unitless/-15-15
troposphericOzBelow13km	Float32	5x35	Ozone below 13 KM	DU/ 0-200
columnAmountOzFirstGuess	Float32	5x35	1 <sup>st</sup> Guess TC Ozone	DU/50-650
columnAmountOzResidualsFirstGuess	Float32	5x35x22	N-Values - 1 <sup>st</sup> Guess TC Ozone Residuals	Unitless/ -100-100
troposphericOzBelow13kmTriplet	Float32	5x35x12	Ozone below 13 KM Triplet	DU/ 0-200
temperatureProfile	Float32	5x35x11	Temperature at Umkher Layers	K/170-350
tropopausePressure	Float32	5x35	Pressure at Tropopause	Atm/0-1.1
snowIceFraction	Float32	5x35	Snow/Ice Fraction	Unitless/0-1
ozProfileForCorr	Float32	5x35x11	Temperature Correction	DU/ 0-200
SOI	Float32	5x35	Sulfur Oxide Index	DU/-12 - 255
surfReflectivity	Float32	5x35	Surface Reflectivity	Unitless/-5-120
columnAmountOzV7	Float32	5x35	TC Ozone	DU/50-650
residualsV7	Float32	5x35x22	Channel residuals using the Version 7 retrieval – N-Values	Unitless/ -100 -100
sensitivitiesV7	Float32	5x35x22	dN/domega values – Sensitivity of N-Values to ozone change	N-Value/DU 0-1
FirstOzoneFromTripletPairs	Float32	5x35x12	1 <sup>st</sup> Guess TC Ozone from triplet pairs	DU/50-650
aerosolCorrOz	Float32	5x35x4	Aerosol Corrected Ozone	DU/50-650
profTempCorrOz	Float32	5x35x4	Temperature Corrected Ozone	DU/50-650
algorithmFlag	Byte	5x35	Indicates which triplet pairs were used in the retrieval	Unitless/1-31
errorFlag	Byte	5x35	Retrieval Quality Flag	Unitless/0-4
Decending/Accending Retrieval	Bit	5x35	Retrieval orbit description	Unitless/0-1
Snow/Ice Present	Bit	5x35	Indicates presence of snow/ice	Unitless/0-1
Tropospheric Aerosols	Bit	5x35	Indicates presence of tropospheric aerosols	Unitless/0-1
Snow/Ice fraction > 0	Bit	5x35	T/F for Snow/Ice	Unitless/0-1
Solar Zenith > 80	Bit	5x35	T/F for SZA > 80 degrees	Unitless/0-1
Ozone Profile w/ Temp/Press correction	Bit	5x35	T/F for availability of ozone profile	Unitless/0-1
CrIMSS Temp Profile Used	Bit	5x35	T/F for use of CrIMSS Temp Profile	Unitless/0-1
VIIRS Snow/Ice	Bit	5x35	T/F for VIIRS Snow/Ice availability	Unitless/0-1
VIIRS CTP QF	Bit	5x35	T/F for VIIRS Cloud Top Pressure	Unitless/0-1
Total Column Quality	2 Bits	5x35	Overall Quality of the Retrieval	Unitless/0-3
Input Data Quality	Bit	5x35	T/F w/r to if input data is bad	Unitless/0-1
Ozone triplet consistency	Bit	5x35	T/F w/r to O3 triplet selection consistency	Unitless/0-1
Residual Consistency	Bit	5x35	T/F w/r to residual consistency	Unitless/0-1
SO2 Index >6DU	Bit	5x35	T/F w/r to SO2 Index	Unitless/0-1
SZA	2 Bits	5x35	SZA w/r to degradation vs exclusion	Unitless/0-2
Snow/Ice QF	Bit	5x35	T/F w/r to snow/ice in FOV	Unitless/0-1

Output	Type	Dimension	Description	Units/Valid Range
Sun Glint QF	Bit	5x35	T/F w/r sun glint	Unitless/0-1
Solar Eclipse QF	Bit	5x35	T/F w/r to evidence of eclipse	Unitless/0-1
TC outside of range	Bit	5x35	T/F w/r to retrieval being outside of range	Unitless/0-1
Performance Range	2 Bits	5x35	Binned TC retrieval	Unitless/0-2
Aerosol Index Exceeded	Bit	5x35	T/F w/r aerosol index threshold	Unitless/0-1
SAA QF	Byte	5	South Atlantic Anomaly Flag	Unitless/0-8

### 2.1.2 Algorithm Processing

The OMPS Total Column (TC) EDR algorithm is derived from the ProCmnAlgorithm class. It is responsible for producing an ozone total column EDR. The algorithm controls, through use of a configuration guide and SI Interfaces, the data flow between operational and science portions of the algorithm and DMS. When the algorithm has finished processing data, an output item is written to DMS that contains all entries for each granule. The original science code had a “glueware” module which remapped the SDR outputs into a format for the IP/EDR to read. This remapping has been moved to C++ modules in the ProEdrOmpsTcUtil.cpp class.

IDPS has two separate processes for computing the Total Column First Guess IP and the EDR. The primary difference between these two processes is the use of external EDR data from the VIIRS and CrIMSS. Cloud Top Pressure is determined from climatology. Cloud Fraction, and Snow/Ice Cover are determined from VIIRS and a Temperature Profile determined from CrIMSS. For the computation of the IP, ancillary data from dynamic sources such as NCEP and static sources such as climatologies are used. The IP is intended to be a primary source of total column ozone for many VIIRS EDRs in NPP and C1 processing during states 2 and 3. Within IDPS, the TC IP will be executed before most VIIRS EDRs and the TC EDR processing will be executed once all requisite VIIRS EDRs are available in the DMS. Both the TC IP and EDR processes utilize the same total column algorithm processing described in this section, but with different input sources.

The purpose of the TC algorithm is to invert nadir radiances to TC ozone and to write the TC EDR data. Total column ozone is derived for each of the 35 50x50km FORs from triplets formed with 22 normalized radiances using the OMPS SDRs and multiple scattering tables as inputs.

The following sections describe the process of how the TC ozone is produced from OMPS total nadir column sensor measurements. Also discussed are assumptions contained in the algorithm, data checks, and assessments that are done in the algorithm.

#### 2.1.2.1 Glueware Modules

The Total Column IP and EDR use a common library to reformat the inputs to pass into the science code. The remapping of inputs common to both the IP and the EDR is done in the sdr\_to\_edr() method. The remapping of inputs that are specific to the IP or the EDR are done in the doProcessing() method of each algorithm. The remapped inputs are shown in **Table 3. TC EDR Bundled Input.**

### 2.1.2.1.1 sdr\_to\_edr Module

The sdr\_to\_edr module is responsible for formatting the majority of the data in the format expected by the science code. This includes such things as converting data from radians to degrees and initializing inputs expected by the science code. The sdr\_to\_edr module also derives the wavelength indices from the actual spectral registration data from the SDR and calculates normalized radiances. Normalized radiances passed to the TC IP and TC EDR algorithms are calculated as follows:

```
tphi = 2*pi*(day_of_year-1)/365;  
esfctr= 1.000110 + 0.034221*cos(tphi) + 0.001280*sin(tphi) + 0.0007189*cos(2*tphi) +  
        0.000077*sin(2*tphi);  
nval[icnt] = -100.0 * log10f(rad / (esfctr*sfl[icnt]));
```

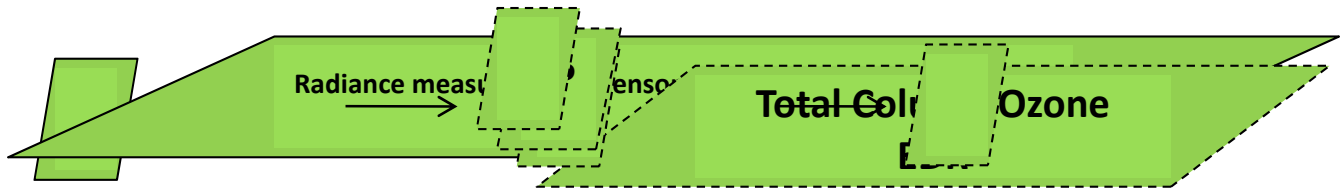
where icnt is the index for each of the 22 wavelengths  
rad and sfl are the radiance and solarFlux, respectively, from the OMPS TC SDR

### 2.1.2.1.2 store\_edr Module

The store\_edr module is responsible for taking the outputs from the science code in the intbuf and realbuf arrays and formatting the data in the format specified by the CDFCB-X. This data is summarized in **Table 7. Total Column Ozone Output File Content** and is fully documented in the CDFCB cited in Section 1.3. The store\_edr module does not do any unit conversions, but does do such things as converting 32-bit integers to 8-bit integers for setting quality flags when copying data into the Data Management System buffer for the TC IP or TC EDR.

### 2.1.2.2 Cross-sensor Modules

The Total Column EDR uses external EDRs from VIIRS and CrIMSS as primary inputs. These external EDRs are not immediately in a format directly usable by the Total Column algorithm. Data is collocated to TC using two high-level steps.



Granule Input	Heap Grid Tile	Heap TC Granulation
VIIRS Cloud Top Parameters IP	Cloud Pressure	Cloud Top Pressure
		Cloud Fraction
VIIRS Snow Cover Depth EDR	Snow/Ice	Snow/Ice Fraction
VIIRS IST EDR		
CrIMSS AVTP IP	Temperature Profile	Combined Temperature Profile

## Granule(s)

**Figure 2: Cross Sensor Concept**

First, EDRs are remapped from native EDR space to a sensor-agnostic space. IDPS has chosen a sinusoidal grid for this purpose. Second, data is remapped from the sinusoidal grids to the appropriate total column FOVs for the tasked granule. See Figure 2 for a list of external EDRs, grids, and the data derived from those grids.

The following subsections describe the approach used to collocate external EDR data to the nadir total column sensor space.

### 2.1.2.2.1 Granule Matchup

Across IDPS, the temporal intervals for granules vary from sensor to sensor. Granule sizes can also change during the mission, so dynamic matchup of granules from the source sensor to the destination sensor is important for robustness. The software makes a series of calls to the INF Granule ID utility using time information for the tasked TC granule. Unique granule IDs for the source sensor are saved for later use. For VIIRS-to-TC and CrIMSS-to-TC matchups, this is expected to be a many-to-1 relationship.



#### **2.1.2.2.2 CrIMSS to Sinusoidal Grid Mapping – Production**

In order to faithfully reproduce the CrIMSS temperature profile in a sinusoidal grid, the relationship of FORs to individual grid cells must be available. Latitude and longitude values are converted to grid cell coordinates to produce a mapping for each matched-up granule that answers the question “For each OMPS grid cell that needs to be updated, which CrIMSS FOR’s data should be used?”

#### **2.1.2.2.3 Update Grids with CrIMSS**

Using the list of granules from 2.1.2.2.1 and the mapping information from 2.1.2.2.2, the CrIMSS temperature profile is vertically averaged from OSS levels to 11 Umkehr layers and stored in 5km x 5km grid cells.

#### **2.1.2.2.4 Update Grids with VIIRS**

To support the VIIRS data needed for the TC EDR, the matched-up granules for one IP and two EDRs are used to update two grids: Snow/Ice and Cloud Pressure

To populate a grid of 1km x 1km cells for Snow/Ice, data from the Snow Cover Depth EDR and IST EDR are used. Finite (non-fill) values from the IST are indicative of sea ice. The presence of either snow or ice causes a snow/ice grid cell to be updated to true. The software uses an Area Weight IP (as created for VIIRS Gridded IPs) with the Greatest Weight Neighbor (GWN) approach for determining which moderate resolution VIIRS pixel(s) should be used to update a grid cell.

To populate a grid for Cloud Top Pressure, data from the non-parallax-corrected Cloud Top Parameters IP is used. The GWN approach is also used.

#### **2.1.2.2.5 TC Granulation of Temperature Profile Grid**

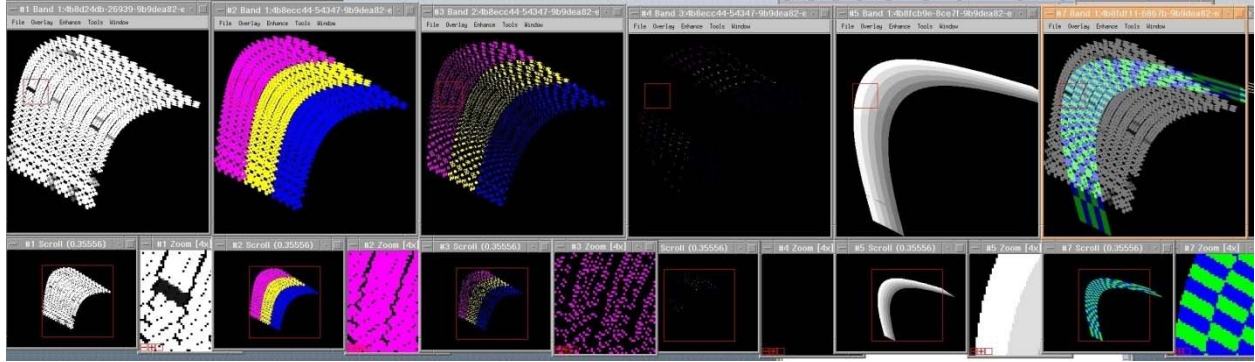
The goal of the temperature profile granulation is to achieve the best value (by preference of source of temperature profile data) in a three dimensional TC space. Due to various limitations, a hybrid profile is created. The CrIMSS does not provide full cross-track coverage for TC space, so ancillary data is used as a supplement. NCEP is preferred over TOMS V8 climatology, but NCEP is vertically limited in that it only provides data useful for the lowest 6 Umkehr layers. See Figure 3 for an understanding of which sources are nominally used for each 3D region of the profile.



**Figure 3: Nominal Combined Temperature Profile for use in TC EDR**

The CrIMSS region is accessed from the newly-created, temporary temperature profile grid. Grid cells are selected based on spatial intersection with a TC FOV polygon that is based on the total column’s corner geolocation. The polygon is fully compatible with the sinusoidal discontinuity of the 180 degree meridian. A combined NCEP and TOMS V8 profile is already granulated in the SDR process. The combined NCEP and TOMS V8 temperature profile is the same profile used as input to the TC First Guess IP process. The TC EDR process favors CrIMSS as a source when available.

In Figure 4 below, several aspects of the cross-sensor granulation are illustrated.



**Figure 4: CrIMSS to TC Visualized**

All images are in sinusoidal grid coordinates. The first image shows the temperature data for the lowest Umkehr profile (Image zooms well and can also be enlarged). The second image uses differently colored density slices to illustrate which grid cells were updated based on FORs from three different CrIMSS granules. Similarly, the third and fourth images show colored pixels where a second or even third pixel was used in averaging to create the grid cells shown in the first image. The fifth image illustrates five swaths in a TC granule. The rightmost image uses a green/blue checkerboard to show the spatial location of individual TC FOVs. These FOVs are overlaid with the data from the first image and truly show which CrIMSS data will be spatially averaged and used in the final TC space. It is easy to see that the TC FOVs on the edge of each swath lack CrIMSS data and falls back to ancillary data as anticipated. Also, some data points from all three coincident CrIMSS granules are used.

It is worth noting that the granule shown in this example is very close to the North Pole and straddles Siberia and the Arctic Ocean. The bowing effect is normal at these latitudes and is a feature of the projection. The individual grid cells are representative of nearly the same surface area regardless of latitude –this is a perk of using this projection.

**2.1.2.2.6 TC Granulation of Cloud Pressure Grid**

The TC granulation of the cloud pressure grid prepares two types of information for use in TC EDR processing. One is a cloud pressure representative of each TC FOV and the other is a cloud fraction.

For the cloud pressure, non-fill grid cells within TC FOV polygon are averaged. For cloud fraction, finite cloud pressure are used to indicate clouds, fill values represent no clouds. If no data is available, the TC EDR will internally compute a cloud fraction, just like the TC IP processing does.

**2.1.2.2.7 TC Granulation of Snow/Ice Grid**

The Snow/Ice grid contains values that indicate snow/ice, no snow/ice, or fill. Non-fill grid cells within the TC FOV polygon are used to determine the fraction of snow/ice cells vs. total non-fill cells. The resulting fraction is used for TC EDR to determine scene conditions.

**2.1.2.3 Main Science Module - calcOTC.f**

The main program **calcOTC.f** performs the following preliminary tasks:

- 1) Scales the normalized radiances passed in from the sdr\_to\_edr Glueware.
- 2) Calculates interpolation factor.
- 3) Determines linear factors needed to interpolate sensor table values between wavelength sets that bracket the wavelength values provided by the SDR.
- 4) Since the denominators of the Lagrange functions  $L_i(X)$  and  $L_j(Y)$  do not depend upon satellite measured quantities, these are computed for each sequential 4-point segment of tabular  $\theta_0$  and  $\theta$  values.
- 5) Sets Raman scattering correction factors to zero for each of the 22 wavelengths.
- 6) Sets pointers to alias actual variables used throughout the program.
- 7) Determines on which side of the CCD the macropixel is located.
- 8) Check to see if the solar zenith angle exceeds 88 degrees. If it does, write out fill values and exit program.
- 9) Calls total.f, which is the main driver for the primary inversion algorithm.

**2.1.2.4 Primary Inversion Subroutine (total.f)**

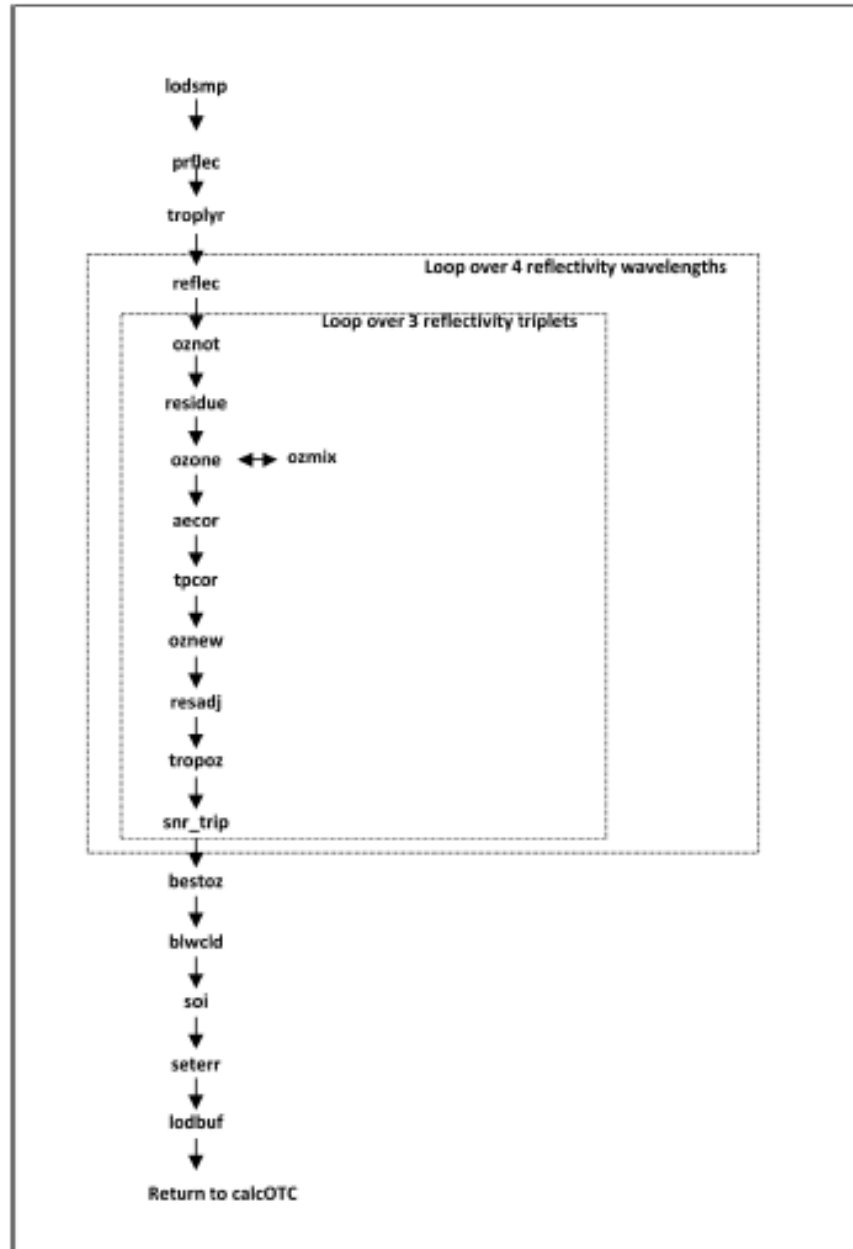
The subroutine **total** is the main driver for the primary inversion algorithm. This subroutine obtains total ozone and determines SO<sub>2</sub> contamination for each OMPS measurement. The flow diagram for total is shown in Figure 5. This flow diagram is a very high-level call graph.

At the top of the subroutine the initial ozone estimate is calculated from the satellite latitude at the beginning of the first scan in the orbit based upon latitude as follows:

$ \text{lat}  < 45^\circ$	$\Omega_{\text{init}} = 260 \text{ DU}$
$45^\circ <  \text{lat}  < 60^\circ$	$\Omega_{\text{init}} = 340 \text{ DU}$
$ \text{lat}  > 75^\circ$	$\Omega_{\text{init}} = 360 \text{ DU}$

The subroutines shown in Figure 5 are then called from **total**. After the call to **ozone** the following is performed in **total**. To account for the change in calculated ozone value, adjust residues using the following formula:

$$r_{adj} = [r_{prf1} \cdot (1 - f_m) + r_{prf} \cdot f_m] - (\Omega - \Omega_{mix}) \cdot \eta$$



**Figure 5: Total Column Ozone Inversion Subroutine total.f**

**2.1.2.5 Subroutine lodsmf.f**

Subroutine lodsmf loads satellite observed quantities and performs the following calculations:

- 1) Unpack  $\theta$ ,  $\theta_0$ ,  $\phi$ , latitude, longitude, and day number.

If  $\theta > 88^\circ$  skip this measurement:

- 2) Set latitude flag for this sample:

$$|\text{lat}| < 15^\circ \quad \text{ILAT} = 1$$

$$45^\circ < |\text{lat}| < 60^\circ \quad \text{ILAT} = 2$$

$$|\text{lat}| > 75^\circ \quad \text{ILAT} = 3$$

- 3) Screen sample for possible contamination by an eclipse.
- 4) Acquire the cloud pressure  $p_c$ , the presence of snow or ice, and the surface category from the SDR. These are either values from external EDRs or, if not available, values from ancillary or gridded IP sources. Acquire the terrain pressure and surface reflectivity as granulated from climatological databases.
- 5) Acquire in radiances for each of the 22 wavelengths.
- 6) Calculate angular quantities necessary to determine calculated N values:  
 $Y = \ln(\sec\theta_0)$ ,  $s = \sec\theta + \sec\theta_0$ ,  $\cos\phi$ ,  $\cos 2\phi$ ,  $Q_1$ , and  $Q_2$ .
- 7) Find the 4 tabular values of  $\theta_{0j}(j=1,1+3)$  that bracket the observed solar zenith angle and determine  $L_j(X)$ ,  $l = 1+3$  (use  $n=4$ ). Do the same for  $L_j(Y)$  using the bracketing values of  $\theta_{0j}(j=k,k+3)$  (also with  $n=4$ ).

### 2.1.2.6 Subroutine prflec.f

Set  $R_t$  = surface reflectivity (from N7/TOMS UV surface ref database) and  $R_c = 0.80$  (cloud reflectivity)

### 2.1.2.7 Subroutine troplyr.f

Calculate the tropopause layer from external EDR temperature information.

### 2.1.2.8 Subroutine reflc.f

For each of the 4 ozone-insensitive reflectivity wavelengths (364, 367, 372, and 377 nm):

- 1) Compute an effective cloud fraction,  $f^*$ , and an effective reflectivity,  $R^*$ .
- 2) Compute the terrain value of the normalized radiance,  $I_t$ , using  $R_t$

$$I_c = I_0 + I_1 \cos\phi + I_2 \cos 2\phi + \frac{R_c T}{1 - R_c S_b}$$

$$I_t = I_0 + I_1 \cos\phi + I_2 \cos 2\phi + \frac{R_t T}{1 - R_t S_b}$$

and the cloud value of the normalized radiance,  $I_c$ , for the 1.0, 0.7, 0.4, and 0.1 atm tables:

Lagrange interpolation is used to obtain the calculated quantities  $I_0$ ,  $Z_1$ ,  $Z_2$ ,  $T$ , and  $S_b$ ;  $I_1$  and  $I_2$  are obtained using  $Z_1$ ,  $Z_2$ ,  $Q_1$ , and  $Q_2$  values calculated in OMPS. A correction for Raman scattering (which is not accounted for in the radiative transfer tables) is applied to the normalized radiance (NR) at all 4 pressure levels and for both  $R_t$  and  $R_c$ .

Lagrange interpolation is then used between the 1.0, 0.7, 0.4, and 0.1 atm parts of the table to obtain  $I_t$  and  $I_c$  for the correct terrain and cloud pressures.

If  $I_{\text{meas}} \leq I_t$  or  $I_t > I_c$ :

- 1) Compute  $R^*$  for the 1.0, 0.7, 0.4, and 0.1 atm tables:

$$R^*(P) = \frac{I_{\text{meas}}^\lambda - I_a^P}{T + S_b (I_{\text{meas}}^\lambda - I_a^P)}$$

where

$$I_a^P = I_0^P + I_1^P \cos \phi + I_2^P \cos 2\phi$$

- 2) Use Lagrange interpolation to determine  $R^*$  for the given terrain pressure.
- 3) Set the cloud fraction,  $f^*$ , equal to 0.
- 4) Set the surface reflectivity,  $R_t$ , to  $R^*$  found in 2).

If  $I_t < I_{meas} < I_c$ :

- 1) Calculate cloud fraction according to:

$$f^* = \frac{I_{meas}^\lambda - I_t}{I_c - I_t}$$

If  $I_{meas} > I_c$ :

- 1) Compute  $R^*$  for the 1.0, 0.7, 0.4, and 0.1 atm tables:

$$R^* = \frac{I_{meas}^\lambda - I_a}{T + S_b(I_{meas}^\lambda - I_a)}$$

where

$$I_a^P = I_0^P + I_1^P \cos \phi + I_2^P \cos 2\phi$$

- 2) Use Lagrange interpolation to obtain  $R^*$
- 3) Set  $f^* = 1$ .
- 4) Set the cloud reflectivity,  $R_c$ , to  $R^*$ .

Subroutines called by **reflec**:

**intnor**: perform table look-ups for the Northern Hemisphere

**intsou**: perform table look-ups for the Southern Hemisphere

**plint**: perform Lagrange interpolations

(Note: the tables for the Northern and Southern Hemisphere are currently the same).

### 2.1.2.9 Subroutine oznot.f

This subroutine computes  $\Omega_0$  using the 318.0/336.0 pair of wavelengths and the partial cloud algorithm. A single set of ozone profiles (low for  $|\text{lat}| \leq 15^\circ$ , mid for  $15^\circ \leq |\text{lat}| \leq 60^\circ$ , high for  $|\text{lat}| \geq 60^\circ$ ) are used.

- 1) Start with the initial guess of ozone appropriate for latitude zone ILAT or, for measurements other than the first one, the result from the previous measurement.
- 2) Using the 1.0 atm tables and  $R_t$  find  $I_0$ ,  $Z_1$  (and, from it,  $I_1$ ),  $Z_2$  (and, from it,  $I_2$ ),  $T$ , and  $S_b$  and calculate  $I_t(1.0 \text{ atm})$ . Apply a correction for Raman scattering (which is not accounted for in the radiative transfer code) to the NR. Do the same thing with the 0.7, 0.4, and 0.1 atm tables. Use Lagrange interpolation on the calculated NRs at the 4 pressure levels to determine  $I_t$  at the terrain pressure. In a similar manner, determine  $I_c$  using the cloud pressure instead of the terrain pressure.

3) Use the cloud fraction,  $f^*$ , calculated in subroutine *reflec* to interpolate between  $I_t$  and  $I_c$  to produce  $I_{calc}$ . Calculate  $N_{calc} = N_{318} - N_{336}$  from  $I_{calc} = I_{318}/I_{336}$ .

4) If  $N_{calc}$  is lower than the measured  $N$  value,  $N_{meas}$ , perform the above calculation for the next higher ozone value in the table, If  $N_{calc}$  is higher than  $N_{meas}$ , go to the next lower ozone value. Continue searching through the profiles in the latitude zone designated by *ILAT* to find the two values of ozone,  $\Omega_L$  and  $\Omega_U$ , whose corresponding pair  $N$  values,  $N_L$  and  $N_U$ , bracket  $N_{meas}$  at the observed solar zenith angle, satellite zenith angle, and azimuth angle and for the reflectivity calculated previously.

5) The ozone amount between 1.0 and 0.4 is contained in a table for each of the 26 profiles. The terrain pressure is used to calculate the fraction of this ozone amount that is below the ground and this amount is subtracted from both  $\Omega_L$  and  $\Omega_U$ .

6) Linearly interpolate to obtain an estimate of ozone for the latitude zone:

$$\Omega_0 = \Omega_L + \frac{N_{meas} - N_L}{dN/d\Omega}$$

where  $dN/d\Omega$  is the ozone sensitivity given by

$$\frac{N_U - N_L}{\Omega_U - \Omega_L}$$

7) Using the procedure above, calculate ozone for two temperature sensitive triplets (including the 316/321 and 318/329 nm pairs).

Subroutines called by **oznot**:

**nvbrac**: determines whether  $N_{calc}$  is above or below  $N_{meas}$  in order to determine bracketing values;

**prfind**: determines profile index (the pointer that indexes the correct profile in the table);

**qvalue**: determines table values. It calls the following subroutines:

**intnor**: performs table look-ups for the Northern Hemisphere

**intsou**: performs table look-ups for the Southern Hemisphere

**plint**: performs polynomial interpolations.

### 2.1.2.10 Subroutine *residue.f*

Compute two sets of residues and sensitivities for wavelengths comprising from two sets of profiles (low and mid for  $|lat| < 45^\circ$ , mid and high otherwise). Also, calculate residues for the 336 nm and 377 nm wavelengths.

1) For each of the two latitude bands and wavelengths, use  $\Omega_0$  to determine  $I_0$ ,  $I_1$  (from  $Z_1$ ),  $I_2$  (from  $Z_2$ ),  $T$ , and  $S_b$  for the 1.0, 0.7, 0.4, and 0.1 atm tables. Using  $f^*$ ,  $R_t^*$ ,  $R_c^*$  and reversing the calculations in subroutine *oznot*, determine  $N_{calc}$ .

2) Calculate residues:

$$r = N_{meas} - N_{calc}$$

3) Calculate the OMPS "aerosol index" ( $R_{336-377}$ ).

Subroutines called by *residue*:

**prfind**: determines profile index (the pointer that indexes the correct profile in the table);

**qvalue**: determines table values. It calls the following subroutines:



**intnor**: performs table look-ups for the Northern Hemisphere  
**intsou**: performs table look-ups for the Southern Hemisphere  
**plint**: performs polynomial interpolations.

**2.1.2.11 Subroutine ozone.f**

Compute a new ozone estimate for each of the 3 wavelength triplets.

- 1) Determine which three triplets to use by calculating the optical path length:

$$somega = \frac{\Omega_{est} \cdot (\sec\theta_0 + \sec\theta)}{1000}$$

- 2) For each of the 3 triplets:

- a. Compute two separate values of  $\Omega$  at two latitudes using the two sets of residues and sensitivities obtained in subroutine residue and the following formula:

$$\Omega_{profile} = \Omega_0 + \frac{r_1\Delta\lambda_2 - r_2\Delta\lambda_1}{\eta_1\Delta\lambda_2 - \eta_2\Delta\lambda_1}; \Delta\lambda_i = \lambda_i - \lambda_R$$

where subscripts refer to two selected wavelengths,  $\eta$  is the sensitivity, and  $r$  is the residue.

- b. To account for the change in calculated ozone value, adjust residues using the following formula:

$$r_{adj} = [r_{prf1} \cdot (1 - f_m) + r_{prf} \cdot f_m] - (\Omega_{profile} - \Omega_0) \cdot \eta$$

- 3) Call **ozmix** to determine select mixing fraction between low- and mid- or mid- and high-latitude profiles.

Subroutines called by **ozone**:  
 ozmix

For somega  $\leq$  1.5, mix  $\Omega$ s to get  $\Omega$  using the latitude mixing fraction,  $f_m$ :

$$\Omega_{mix} = (1 - f_m) \cdot \Omega_{prf1} + f_m \cdot \Omega_{prf2}$$

where prf1 and prf2 are low- and mid- or mid- and high-latitude profiles, respectively, and

$f_m = 0$	for $ \text{lat}  \leq 15^\circ$ ,
$f_m = ( \text{lat} -15)/30$	for $15^\circ <  \text{lat}  < 45^\circ$ ,
$f_m = ( \text{lat} -45)/30$	for $45^\circ <  \text{lat}  < 75^\circ$ , and
$f_m = 1$	for $ \text{lat}  \geq 75^\circ$ .

For somega  $>$  1.5 **AND**  $R_{336-377} >$  1, use the following procedure:

- 1) For each triplet chosen in subroutine ozone, use a 4<sup>th</sup> wavelength that is sensitive to ozone profile shape to select mixing fraction between low- and mid- or mid- and high-latitude profiles. For example, if the optical path length of the measurement is 1.7, the 3

Triplets chosen in subroutine ozone are formed by using one of the 4 reflectivity wavelengths with the 312.5/321.0, 314.0/321.0, and 318.0/336.0 nm pairs. For these 3 triplets, the 308.5 nm wavelength is used to select ozone profile shape.

- 2) Calculate a residue for the 4<sup>th</sup> wavelength,  $r_4$ .
- 3) For each of the two profile sets, calculate the “triplet residue”:

$$r_{trip} = r_4 - r_2 \frac{\lambda_4 - \lambda_R}{\lambda'_2 - \lambda_R}$$

where  $r_2$  is the middle wavelength of the wavelength triplet.

- 4) Calculate the mixing fraction (limit it to be between -.5 and 1.5):

$$f_m = \frac{r_{trip}(lower)}{r_{trip}(lower) - r_{trip}(higher)}$$

If  $f_m > 1.5$  then  $f_m = 1.5$

If  $f_m < -.5$  then  $f_m = -.5$

- 5) Calculate ozone using this mixing fraction:

$$\Omega_{mix} = (1 - f_m) \cdot \Omega_{prf1} + f_m \cdot \Omega_{prf2}$$

and readjust residues

$$r = [r_{prf1} \cdot (1 - f_m) + r_{prf2} \cdot f_m] - (\Omega_{mix} - \Omega_0) \cdot \eta$$

- 6) Recalculate  $r_{trip}$ . If it is greater than 0.1, iterate once using  $\Omega_{mix}$  determined in 4 above.

$\Omega_{mix}$  corresponds to the heritage V7 ozone amount,  $\Omega_{V7}$ .

### 2.1.2.12 Subroutine aecor.f

This subroutine corrects  $\Omega_{mix}$  for tropospheric aerosols and sea glint.

$$\begin{aligned} \Omega_{aecor} &= \Omega_{V7} + 0.75 R_{336-377} - 0.011 R_{336-377}^2 \text{ for } PL \leq 4.5 \\ \Omega_{aecor} &= \Omega_{V7} + 0.80 R_{336-377} \text{ for } PL > 4.5 \end{aligned}$$

Convert to aerosol index using equation below and report out:

$$Aerosol\ Index = \frac{331 - 360}{336 - 377} R_{336-377}$$

### 2.1.2.13 Subroutine tpcor.f

This subroutine corrects for differences between the actual ozone and temperature profiles and standard ozone and temperature profiles.

- 1) Calculate  $dN/dx$  and  $dN/dt$  using the  $dN/dx$  sensitivity table.

**Unperturbed Profile**

For each of the two latitude bands and wavelengths, use  $\Omega_{aerCor}$  to determine  $I_0$ ,  $I_1$  (from  $Z_1$ ),  $I_2$  (from  $Z_2$ ),  $T$ , and  $S_b$  for the 1.0, 0.7, 0.4, and 0.1 atm  $dN/dx$  tables. Use the following formula to determine  $dn/dt$  from  $dn/dx$ :

$$\sum_x \left( \frac{\Delta N}{\Delta T} \right)_x = \sum_x \left( \frac{\partial N}{\partial x} \right)_x \frac{x}{\alpha_x} \frac{\partial \alpha}{\partial T} = \sum_x \left( \frac{\partial N}{\partial x} \right)_x \frac{x}{\alpha_x} \left[ \alpha(T_x^{stdprf}) - \alpha(T_x^{measured}) \right]$$

where

$$\alpha = c_0 + c_1 T + c_2 T^2$$

and  $c_0$ ,  $c_1$ ,  $c_2$  are located in the file `abs_coef.dat` as a function of wavelength.

$T^{measured}$  for each layer is obtained from the external EDR.

Using  $f_m$ ,  $f^*$ ,  $R_t^*$ ,  $R_c^*$  and reversing the calculations in subroutine `oznot`, determine  $N_{calc}$ .

**Perturbed Profiles**

For each of the two latitude bands and wavelengths, use  $\Omega_{V7}$  to determine  $I_0$ ,  $I_1$  (from  $Z_1$ ),  $I_2$  (from  $Z_2$ ),  $T$ , and  $S_b$  for each of the 11 perturbed profiles for the 1.0, 0.7, 0.4, and 0.1 atm  $dN/dx$  and  $dN/dt$  tables. Again, use  $f_m$ ,  $f^*$ ,  $R_t^*$ ,  $R_c^*$  and reverse the calculations in subroutine `oznot` to determine  $N_{calc}$  for each of the perturbed profiles.

- 2) Using  $N$  values calculated for the unperturbed profile and the  $N$  values calculated for the perturbed profiles, calculate 11  $dN/dx$  and  $dN/dT$  values (one for each of the 11 layer perturbations).
- 3) Using  $\Omega_{aerCor}$  and  $f_m$ , determine the standard ozone and temperature profile used in the table lookup.
- 4) Use the EDR external temperature profile to determine the difference between the actual and standard temperature,  $\Delta t$ , for all 11 layers.
- 5) Use an actual ozone profile to determine the difference between the actual and standard ozone profile,  $\Delta x$ , for all layers for which there is an actual retrieval.
- 6) Form the two sums:

$$\sum_{layer} (t_{layer} - t_{layer}^0) \frac{dN}{dt_{layer}}$$

$$\sum_{layer} (x_{layer} - x_{layer}^0) \frac{dN}{dx_{layer}}$$

Calculate  $dxerr$  (error in ozone profile shape correction) and  $dterr$  (error in temperature shape correction (to be used in weighted average to obtain final ozone amount))

Subroutines called by `tpcor`:

- prfind**: determines profile index (the pointer that indexes the correct profile in the table);
- qvalue**: determines table values

**qvprof:** calculates q values. It calls the following subroutines:  
**intlyrn:** computes q values for selected lambda using the dn/dt table for the Northern Hemisphere.  
**Intsou:** computes q values for selected lambda using the dn/dt table for the Southern Hemisphere.

**2.1.2.14 Subroutine oznew.f**

Subroutine **oznew** forms the equation

$$r = N_m - N_{aercor} = (\Omega - \Omega_{aercor})\eta + \sum_{layer} (t_{layer} - t_{layer}^0) \frac{dN}{dt_{layer}} + \sum_{layer} (x_{layer} - x_{layer}^0) \frac{dN}{dx_{layer}} + a + b\lambda$$

and then solves for  $\Omega$ :

$$\Omega_{cor} = \Omega_{aercor} + \frac{r_1 \Delta\lambda_2 - r_2 \Delta\lambda_1}{\eta_1 \Delta\lambda_2 - \eta_2 \Delta\lambda_1}.$$

**2.1.2.15 Subroutine resadj.f**

To account for the change in calculated ozone value, adjust residues using the following formula:

$$r_{adj} = [r_{prf1} \cdot (1 - f_m) + r_{prf} \cdot f_m] - (\Omega - \Omega_{aercor}) \cdot \eta$$

**2.1.2.16 Subroutine tropoz.f**

Calculate the climatological amount of tropospheric ozone in standard profile used to determine  $\Omega$  down to 13 km.

1) Calculate efficiencies for layers below 13 km:

$$\xi_{layer} = \frac{dN_{triplet}/dx}{dN_{triplet}/d\Omega}$$

where the numerators are obtained from subroutine tpcor and the denominators are obtained from subroutine ozone.

2) Calculate the amount of retrieved ozone below 13 km and subtract the amount from the standard profile corresponding to  $\Omega_{cor}$ .

$$X_{13} = \Omega_{cor} - \sum_{13}^{60} x_{limb} - X_{13}^0$$

3) Use the values above to correct ozone for measurement inefficiency below 13 km:

$$\Omega = \Omega_{cor} - X_{13}^0 + X_{13} = \Omega_{tpcor} + (1 + \xi) \frac{X_{retr} - X_{13}^0}{\xi}$$

4) Calculate troperr (to be used in weighted average to get final ozone amount)

Subroutine called by tropoz:

**prfind:** determines profile index (the pointer that indexes the correct profile in the table)

**2.1.2.17 Subroutine snr\_trip.f**

Calculate the snr error for the triplet from the following formula:

$$\frac{\sigma_{\Omega}}{\Omega} = \sqrt{\frac{(\lambda_2 - \lambda_3)^2 e_1^2 + (\lambda_1 - \lambda_3)^2 e_2^2}{[(\lambda_2 - \lambda_3)s_1 - (\lambda_1 - \lambda_3)s_2]^2}}$$

where  $e_n$  is the normalized standard deviation of the albedo random noise.

**2.1.2.18 Subroutine bestoz.f**

Calculate best ozone from a weighted average of all of the triplets, using snrerr, dxerr, dterr, and troperr using the following formulas:

$$\Omega_{best} = \frac{\sum_i W_i \Omega_i}{\sum_i W_i} \quad \text{where } i \text{ is a triplet value}$$

$$\Delta\Omega_i = \sqrt{snrerr^2 + dterr^2 + dxerr^2 + troperr^2}$$

- 1) Calculate best reflectivity by averaging together reflectivity amounts from 4 reflectivity wavelengths.
- 2) Calculate best aerosol index from a weighted average of all of the triplet values using snrerr, dxerr, dterr, and troperr.

**2.1.2.19 Subroutine blwcl.d.f**

Calculate ozone beneath the cloud for both appropriate latitude bands.

1a) If the cloud pressure is greater than 0.5 atm, the cloud is in layer 1. Determine the fraction of ozone in layer 1 that is below the cloud for the bracketing ozone values (since pressure scales with height exponentially use logarithmic interpolation):

$$f_{cloud} = \frac{\log(1.013 / p_{cloud})}{\log(1.013 / 0.5)}$$

$$\Omega_{cld}^{prflo} = f_{cloud} \cdot \Omega_{layer1}^{prflo}$$

$$\Omega_{cld}^{prfhi} = f_{cloud} \cdot \Omega_{layer1}^{prfhi}$$

1b) If the cloud pressure is less than 0.5, the cloud is in layer 2 (which ends at 0.253 atm). Determine the fraction of ozone in layer 2 that is below the cloud and add to the ozone in layer 1 (which is totally below the cloud):

$$f_{cloud} = \frac{\log(0.5 / p_{cloud})}{\log(0.5 / 0.253)}$$

$$\Omega_{cld}^{prflo} = f_{cloud} \cdot \Omega_{layer2}^{prflo} + \Omega_{layer1}^{prflo}$$

$$\Omega_{cld}^{prfhi} = f_{cloud} \cdot \Omega_{layer2}^{prfhi} + \Omega_{layer1}^{prfhi}$$

2) Mix ozone below cloud from bracketing profiles for the two latitude bands:

$$f_{\Omega} = \frac{\Omega - \Omega_{prflo}}{\Omega_{prfhi} - \Omega_{prflo}} = \frac{\Omega - \Omega_{prflo}}{50},$$

$$\Omega_{cld}^{lat} = \Omega_{cld}^{prflo} \cdot (1 - f_{\Omega}) + \Omega_{cld}^{lat2} \cdot f_{\Omega}.$$

3) Mix  $\Omega_{cld}$  using the profile mixing fraction:

$$\Omega_{cld} = (1 - f_m) \cdot \Omega_{cld}^{lat1} + f_m \cdot \Omega_{cld}^{lat2}.$$

4) Finally, multiply by the cloud fraction:

$$\Omega_{cld} = f_{cld} \cdot \Omega_{cld}.$$

Subroutine called by blwcd:

**prfind:** determines profile index (the pointer that indexes the correct profile in the table)

**2.1.2.20 Subroutine soi.f**

This subroutine determines if SO<sub>2</sub> is present.

For each reflectivity wavelength:

- 1) Calculate the ratio, Rat, of ozone to SO<sub>2</sub> absorption coefficients for the 317, 331 and 336 nm wavelengths.
- 2) Calculate SO<sub>2</sub> sensitivities:

$$\frac{dN}{d(SO_2)} = Rat \cdot \frac{dN}{d\Omega}$$

- 3) Calculate the SO<sub>2</sub> index using

$$SO_2 = \frac{r_{23} \cdot s_{13} - r_{13} \cdot s_{23}}{so_{23} \cdot s_{13} - so_{13} \cdot s_{23}},$$

where

$$s_{13} = \left( \frac{dN}{d\Omega} \right)_{317.0} \cdot (336.0 - \lambda_R) - \left( \frac{dN}{d\Omega} \right)_{336.0} \cdot (317.0 - \lambda_R),$$

$$s_{23} = \left( \frac{dN}{d\Omega} \right)_{331.0} \cdot (336.0 - \lambda_R) - \left( \frac{dN}{d\Omega} \right)_{336.0} \cdot (331.0 - \lambda_R),$$

$$so_{13} = \left( \frac{dN}{dSO_2} \right)_{317.0} \cdot (336.0 - \lambda_R) - \left( \frac{dN}{dSO_2} \right)_{336.0} \cdot (317.0 - \lambda_R),$$

$$so_{23} = \left( \frac{dN}{dSO_2} \right)_{331.0} \cdot (336.0 - \lambda_R) - \left( \frac{dN}{dSO_2} \right)_{336.0} \cdot (331.0 - \lambda_R),$$

$$r_{13} = r_{317.0} \cdot (336.0 - \lambda_R) - r_{336.0} \cdot (317.0 - \lambda_R), \text{ and}$$

$$r_{23} = r_{331.0} \cdot (336.0 - \lambda_R) - r_{336.0} \cdot (331.0 - \lambda_R).$$

- 4) Average the 4 reflectivity wavelengths to obtain the final SO<sub>2</sub> value. Rename SOI and use to flag data if larger than 4σ.

### 2.1.3 Graceful Degradation

#### 2.1.3.1 Graceful Degradation Inputs

The OMPS TC EDR algorithm is based on Version 7 of the Total Ozone Mapping Spectrometer (TOMS) algorithm. A series of enhancements were designed to bring the performance of the heritage algorithm to within the NPOESS specifications. Most of these design enhancements require ingesting external EDR data from the other sensors. This data is collocated in time and space and is matched in terms of the FOV. The OMPS TC EDR algorithm assumes that these operations have been performed (cross-sensor modules) before the data is ingested.

The external EDR data needed by the algorithm, and the sensor supplies this data, are:

- Temperature profile – CrIMSS temperature profile EDR (Block 1) and NCEP (Block 2)
- Cloud top pressure – VIIRS cloud pressure EDR – This information is not used, but is still needed to avoid algorithm failure. – The data is overwritten with the UV climatology information.
- Snow/ice cover – VIIRS snow, ice, and fresh-water ice EDR

If external EDR data from a given NPOESS sensor are not available, the algorithm still retrieves a total column EDR, but with degraded performance. In case 1 above, the algorithm ingests NCEP temperature profile data for the lower 6 Umkehr layers and TOMS V8 Climatology for the upper Umkehr layers. Note that in Block 1, the product will not be marked as degraded when the CrIMSS temperature profile is missing. In case 2 above, the algorithm simply ingests climatological values. FOV level flags are passed through the EDR algorithm and ultimately provided for use by the calibration/validation team and other end users.

The algorithm performs the following actions in the case that a given external value is not available (along with an estimate on the effect to accuracy and precision for the retrieved ozone values):

- If the CrIS pressure profile EDR is not available, the algorithm obtains the terrain pressure from a 0.5° x 0.5° grid terrain pressure database delivered with the algorithm. The lack of pressure information from CrIS, and the use of the terrain height database, results in an increase in the precision error of approximately 0.3% total ozone amount.
- If the CrIMSS temperature profile EDR is not available, the algorithm turns off the temperature profile shape correction. If this correction is turned off, the resulting change in both the accuracy and precision error is approximately 0.2% total ozone amount (the effect of not having the temperature profile to perform this correction is mitigated by the fact that temperature-insensitive wavelengths are used in the retrieval).
- If the cloud top pressure EDR is not available, the algorithm obtains cloud top pressure from a 1° x 1° x 12 month grid of climatological values that were determined from ISCCP data and that was delivered with the algorithm. The use of this database increases both accuracy and precision errors by 0.755 to 1.0% total ozone amount.
- If the snow/ice cover EDRs are not available, the algorithm obtains snow/ice information from a 1km x 1km rolling gridded IP of Snow/Ice cover values from the last high quality observation made by one or many VIIRS sensors (Updated by multiple VIIRS sensors in states 2 and 3 once calibrated). With the exception of latitude and SZA exclusions, the data in this gridded IP is typically updated once a day near the equator and very frequently at latitudes closer to the poles. The use of this database slightly increases the



likelihood of miscalculating surface effects and can lead to large errors in individual retrievals. The effect on overall accuracy and precision, however, is hard to estimate.

Because the OMPS limb-retrieved stratospheric profile is not available, both the ozone profile shape correction and the tropospheric ozone correction are turned off by default.

If no external data are available for use by the OMPS TC EDR algorithm, the performance essentially reverts to the performance of the V7 TOMS algorithm. For more details on the TC EDR accuracy and precision error estimates, consult the OMPS Total Column ATBD, 474-00029. Table 8 below is a Nomenclature cross-reference.

**Table 8. Correlation of OAD, Config Guide, and PowerPoint Terminology**

OAD	Config Guide – First Use	PowerPoint – TC IP	PowerPoint - TC EDR
pcloud	OMPS-TC-ANC-Cd-Top-Press-Gran	Granulated Ancillary Cloud Top Pressure	VIIRS Cloud Top Pressure EDR
vcf	OMPS-TC-CS-GridIP-VIIRS-Cloud-Frac-Gran	Zero Fill	VIIRS Cloud Top Parameters IP
prfoz	OMPS-TC-EDR-LUT	TOMS V8 Ozone Climatology	
vsfrac	OMPS-TC-GridIP-VIIRS-Snow-Ice-Fraction-Gran	Ice Fraction Granulation	VIIRS Snow and VIIRS IST EDR
prftemp	OMPS-TC-ANC-Temp-Press-Lay-Gran	Granulated Ancillary Temperature Pressure At Layers	CrIMSS Temperature Profile EDR
pteran	OMPS-TC-ANC-Press-Surf-Gran	Granulated Ancillary Surface Pressure	
sref	OMPS-TC-ANC-UV-Surf-Reflect-Gran	Granulated UV Surface Reflectance Climatology	

**2.1.3.2 Graceful Degradation Processing**

None

**2.1.3.3 Graceful Degradation Output**

None

**2.1.4 Exception Handling**

Pre-processing screening of input radiances, observational angles, satellite attitude information and sensor status is done within the SDR algorithm. During EDR processing, data quality flags are broken into two categories: geophysical conditions of interest to the scientific/operational community that do not degrade data quality; and those that do degrade data quality. Although not part of the delivered code, we describe in the paragraphs below, error handling for both the SDR and EDR algorithm.

**2.1.4.1 SDR Algorithm**

Before measured NRs are accepted for use in ozone determination, the solar zenith angle, satellite attitude, and instrument status are checked to ensure the suitability of the NRs and

other geophysical input to the algorithm. If the solar zenith angle is greater than 88 degrees EDR processing is not performed.

Using the geolocation data for the beginning and end of each observation, the SDR algorithm checks the ground track of the satellite during an observation and compares it with a static SAA map of relative radiation exposure. The algorithm flags each swath according to the percentage of expected exposure. For example, if the calculated exposure is 45% the data are flagged as exceeding 40% but not 50%. Flagging in 10% exposure gradations with an 80% maximum is adequate, so results are conveniently packed in an 8 bit word.

The algorithm also performs transient pixel detection by comparison with nearest neighbors. A cubic spline, or similar smooth regression, is performed along each row  $J$  (i.e. spectrally) for each data cell. The splined region should not exceed 2 nm. A graded flag, similar to that used for the SAA, is used to indicate the percent by which the measured radiance exceeds that computed from the spline. Macropixels that have lower than expected radiances are not flagged by this algorithm.

Using an almanac of Solar eclipses by the moon, the algorithm checks the latitude and longitude of the Earth data for the presence of a solar eclipse at each Earth spatial cell. If the FOV lies within an eclipse, the algorithm flags the FOV for eclipses and EDR processing is not performed.

Specular reflections of sunlight off water surfaces are a geophysical situation not properly incorporated in the EDR radiance tables. When the sun glint condition is met, water reflects much of the solar irradiation at a solar zenith angle  $\theta_o$  into the sensor field of view at a satellite zenith angle  $\theta$ . Waves diffuse the reflection, creating a range of angles for which sun glint produces an error. This includes reflections out of the principal plane, i.e. relative azimuth angle  $\varphi \neq 0^\circ, 180^\circ$ . The SDR Algorithm checks for sun glint using the following equation for the co-scattering angle  $\Phi$ .

$$\Phi = \cos^{-1}[(\cos \theta_o \cos \theta + \sin \theta_o \sin \theta) \cos \varphi] \leq 30^\circ$$

The algorithm identifies the surface type as water using the surface category stored in the Quarterly Surface Type gridded IP. The glint flag is set when the condition in equation above is met and water covers at least 25% of the FOV.

The SAA, Eclipse, and Sun Glint flags, as determined by the SDR algorithm, are passed to the EDR algorithm.

#### 2.1.4.2 EDR Algorithm

The TC ozone algorithm contains a validity check for maintaining data quality:

- When ozone column estimates fall outside of the [0,650 DU] range and this is not the first iteration in the calculation, the code issues a debug type error message and ends the retrieval.

The TC ozone algorithm contains several validity checks for maintaining data quality. After these checks are applied, quality checks are performed to identify invalid and lower quality

ozone values (outside of the [50, 650 DU] range) caused either by bad input data that passed preprocessing checks or by limitations of the ozone algorithm.

The principal tool used to investigate the validity and quality of a total ozone value is the set of residues. The residues measure how well NRs calculated based on the ozone derived using a set of triplets match the NRs measured at other wavelengths. The usual significance of a large residue is that the atmospheric or surface conditions deviate significantly from those assumed in the algorithm, for example, if reflectivity has a non-linear dependence on wavelength. The final triplet residues for wavelengths used in the retrieval will be zero.

The first check is of all the non-zero residues; if any is greater than 12.5 in units of N-value, then the retrieval should be flagged as bad. This condition usually arises when problems in the data stream lead to incorrect values for the measured NR or when the atmospheric conditions are so unusual that the assumptions used in the calculation of NRs do not hold.

Data that pass the above flag are checked for volcanic sulfur dioxide contamination. The SO<sub>2</sub> Index (SOI) is defined in Section 2.4.11 of the OMPS NADIR Total Column Ozone Algorithm Theoretical Basis Document ATBD, 474-00029. The flag indicating contamination with SO<sub>2</sub> is based on the 1-sigma value of the SOI calculated for a day's worth of OMPS data taken when no volcanic SO<sub>2</sub> is present. If the value of the SOI is larger than the 4-sigma of this value, the data is flagged as being contaminated.

The next check assesses triplet consistency. If the ozone value from any of the 12 triplet retrievals is outside of 3-sigma obtained from the 12 triplet values the retrieval is flagged as suspect.

Another set of flags is set indicating that the following conditions are present for the retrieval. Note that the following flags DO NOT indicate the retrievals are degraded in quality.

- The retrieval is located within the South Atlantic anomaly. This flag should also indicate the approximate level of effect (10%, 20%, etc).
- The retrieval is performed when the surface is covered with snow or ice.
- The retrieval is performed for conditions containing absorbing tropospheric aerosols. This flag should be set if the aerosol index is 0.5 or greater.
- The retrieval is performed for viewing conditions containing sea glint. This flag is set based on geometrical calculations. The retrieval is performed for solar zenith angles above 80 degrees. Although the performance requirements for the OMPS total column sensor-algorithm system are only valid up to 80 degrees, the algorithm performs retrievals up to 88 degrees.
- A flag is set to indicate whether the retrieval is made on an ascending or descending portion of an orbit.
- If the surface reflectivity is a fill value, the retrieval is not performed and a fill value is indicated.

Finally, a set of flags should indicate the following conditions. Note that the following flags DO indicate the retrievals are degraded in quality.

- External temperature profile EDR from CrIMSS was not available for all Umkehr layers for an FOV.

- External cloud pressure EDR from VIIRS was not available for an FOV.
- External snow/ice EDR from VIIRS was not available for an FOV.

#### 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.

### 2.1.5 Computational Precision Requirements

Because the OMPS TC EDR algorithm is based on an older heritage algorithm, it is coded to use single precision ('real' and 'integer') declared variables. Double precision real variables or long integers are not required for computational accuracy.

### 2.1.6 Algorithm Support Considerations

#### 2.1.6.1 Numerical Computation Considerations

Although the TC EDR algorithm contains several iterative loops, the algorithm is not computationally intensive. Double precision computations are not required.

#### 2.1.6.2 Software Environment Considerations

Fortran90 and C++ compilers are necessary to compile the source code for the TC IP/EDR Algorithm and supporting modules.

#### 2.1.6.3 SOI Future Development

The algorithm currently uses a set of SO<sub>2</sub> absorption cross-sections interpolated from TOMS values. The channel averaged absorption cross-sections must be recalculated for OMPS specific wavelengths and spectral bandpasses.

#### 2.1.6.4 Instrument Table Updates

When updating the instrument table for the northern or southern hemisphere, corresponding updates must also be made to the dndx table.

### 2.1.7 Assumptions and Limitations

#### 2.1.7.1 Assumptions

All necessary data will be available and provided within the necessary time constraints.

#### 2.1.7.2 Limitations

None.

### **2.1.7.2.1 ATBD - Operational Adaptation, Deviation or Limitations**

The Algorithm Theoretical Basis Document (ATBD) includes a complete description of methodology the science code uses to calculate total ozone. The delivered science is aligned with the ATBD except for the areas identified in this document. The SO<sub>2</sub> absorption cross-sections must be replaced with cross-sections calculated with updated high resolution cross-sections convolved with the OMPS spectral functions at the OMPS wavelengths. Data output at the end of the Main Science Module - calcOTC.f consists of updating the OMPS TC EDR buffer retrieved from the Data Management Subsystem (DMS) with a real and integer array of variables containing such quantities as total column ozone and other variables related to the atmospheric state and observational conditions.

### 3.0 GLOSSARY/ACRONYM LIST

#### 3.1 Glossary

**Table 9. 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: A theoretical description (i.e., science/mathematical basis) A computer implementation description (i.e., method of solution) 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	Science-grade software delivered by an algorithm provider is verified for compliance with data quality and timeliness requirements by Algorithm Team science personnel. 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)	<p>[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.</p> <p>[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.</p>
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)	<p>[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.</p> <p>[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.</p>
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]

TERM	DESCRIPTION
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 10. 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 11. List of OAD TBDs/TBRs**

<b>No.</b>	<b>DESCRIPTION</b>	<b>PAGES AFFECTED</b>
None		