EUMETSAT

GOME-2 Level 1: Product Generation Specification

Doc.No. : EPS.SYS.SPE.990011
Issue : v8
Date : 8 August 2014

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Dcument Change Record

Issue / Revision	*Date*	*DCN. No*	*Changed Pages / Paragraphs*
Issue 1/ Draft E	04/05/1999		• Based on the AVHRR/3 DRAFT E document structure • Included some known GOME-2 instrument characteristics
Issue 1/ Draft F	07/07/1999		CGSRD RID implementation
Issue 1/ Draft G	15/04/2000		Nearly complete revision based on documentation available through GOME-2 GPP development
Issue 2/ Draft A	28/06/2000		Revision of all current algorithms and work breakdown based on GOME-2 ATBD from GOME-2 GPP development. Addition of requirements Chapter 5.
Issue 2/ Draft B	11/06/2000		Setup new format, in line with other PGSs.
	12/06/2000		Reworded Introduction section in line with new format and clarifying stability of document.
Issue 3/ Draft A	15/11/2000	DCN.SYS.DCN.022	Restructuring of document.
Issue 4/ Revision 0	01/6/2001		Reorganisation of processing logic. Stray light calculation moved to Level 1a to 1b for main channels. • Refinement and increased level of detail for all algorithms in Chapter 5. • Re-numbering and organisation of requirements in Chapter 4 for consistency with the reorganisation in Chapter 5.
Issue 5: 0	17/5/2002		CHAPTER 1 • Applicable document [AD6] in Issue 4 Revision 0 removed • Reference documents - Issue numbers corrected • Reference documents [RD11], [RD12], [RD23] and [RD24] added in Issue 5: 0 • Minor text modifications and clarifications CHAPTER 2 • Information on reference frames moved to Appendices • Minor text modifications and clarifications CHAPTER 3 • Text significantly simplified and revised to reflect the GOME-2 PGF processor interfaces accurately • Figures 3 and 4 in Issue 5: 0 revised to reflect GOME-2 PGF processor interfaces and processing logic accurately • Table 2 in Issue 5: 0 revised CHAPTER 4 • Table 3 containing a description of GOME-2PGF sub-components is revised. This table is provided for reference with respect to the requirements listed in chapter 4. • Changes to requirements: ALG-HGH-005- *revised* ALG-HGH-010- *revised*

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			ALG-HGH-015- *revised* ALG-HGH-025- *revised* ALG-HGH-030- *revised* ALG-HGH-035- *revised* ALG-HGH-040- *revised* ALG-HGH-050- **deleted** ALG-FCT-004- added ALG-FCT-005- *revised* ALG-FCT-006- added ALG-FCT-007- added ALG-FCT-010- **deleted** ALG-FCT-015- **deleted** ALG-FCT-020- **deleted** ALG-FCT-025- *revised* ALG-FCT-026- added ALG-FCT-027- added ALG-FCT-028- added ALG-FCT-030- *revised* ALG-FCT-031- added ALG-FCT-035 added ALG-FCT-036 added ALG-FCT-040- *revised* ALG-FCT-041- added ALG-FCT-042- added ALG-FCT-043- added ALG-FCT-045- *revised* ALG-FCT-046- added ALG-FCT-050- *revised* ALG-FCT-051- added ALG-FCT-052- added ALG-FCT-053- added ALG-FCT-055- *revised* ALG-FCT-056- added ALG-FCT-075- *revised* ALG-FCT-080- **deleted** ALG-FCT-085- *revised* ALG-FCT-090- *revised* ALG-FCT-091- added ALG-FCT-095- *revised* ALG-FCT-100- *revised* ALG-FCT-105- *revised* ALG-FCT-110- *revised* ALG-FCT-115- *revised* ALG-FCT-116- added ALG-FCT-120- *revised* ALG-FCT-125- *revised* ALG-FCT-130- *revised* ALG-FCT-131- added ALG-FCT-135- *revised* ALG-FCT-136- added ALG-FCT-140- *revised* ALG-FCT-145- *revised*

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			ALG-FCT-150- *revised* ALG-FCT-160- *revised* ALG-FCT-170- *revised* ALG-FCT-175- *revised* CHAPTER 5 • All clarifications arising from Algorithm Panel meetings have been introduced • Introductory text and definitions have minor modifications only The abbreviation 'aux' referring to auxiliary inflight calibration data has been replaced with 'ifc' referring to in-flight calibration data, to avoid confusion with other types of auxiliary data • Receive and Validate Level 0 and Auxiliary Data (A1) revised and expanded • Level 0 to 1a Processing (A2) overview modified to focus on interfaces • Figures 5, 5a, 5b and 5c in Issue 5: 0 updated to accurately reflect processor flow as described in algorithm specification sections • Read Input Data (A2.0) specification added including a complete list of input data required by the Level 0 to 1a Processing (A2)
		MO-DCP-GMV-GO-0001	Preprocess Müller Matrix Elements (A2.1) changed so that MMEs are now interpolated to a fixed wavelength grid, **not** the wavelength grid of the current SMR spectrum • Convert Housekeeping Data (A2.2) moved before Determine Observation Mode and Viewing Angles (A2.3) • Determine Observation Mode and Viewing Angles (A2.3) revised to include determination of UTC time grid • Determine PCDs from Raw Intensity (A2.4) added • Calculate Geolocation for Fixed Grid (A2.6) is a substantially revised version of the previous Calculate Geolocation. Geolocation parameters in the Level 0 to 1a Processing (A2) are now calculated on a fixed 0.1875ms time grid. Geolocation parameters for the actual integration time are calculated in Level 1a to 1b Processing (A3). Information on reference frames has been moved to the Appendices Determine PCDs from Geolocation (A2.7) added • Normalise Signals to One Second Integration Time (A2.10) moved as a separate module prior to Calculate PPG (A2.11) • Calculate Spectral Calibration Parameters for PMD Channels (A2.14) significantly revised • Determine Stokes Fractions (A2.21) significantly revised and clarified • Collect Global PCDs per Product (A2.22) added • Write Level 0 and 1a Product (A2.23) added Level 1a to 1b Processing (A3) overview modified to focus on interfaces • Figures 9, 9a, 9b and 9c in Issue 5: 0 updated to accurately reflect processor flow as described in algorithm specification sections • Read Input Data (A3.0) added including a complete

Issue / Revision	Date	DCN. No	Changed Pages / Paragraphs
			list of input data required by the Level 1a to 1b Processing (A3) • Calculate Geolocation for Actual Integration Times (A3.2) added • Normalise Signals to One Second Integration Time (A3.4) moved as a separate module prior to Calculate PPG (A2.11) • Apply Polarisation Correction (A3.10) significantly revised paying particular attention to the synchronisation between main channel and PMD readouts • Calculate Fractional Cloud Cover and Cloud Top Pressure (A3.15) moved to Level 1a to 1b Processing (A3) and completely specified • Collect Global PCDs per Product (A3.16) added • Write Level 1b Product (A3.17) added • Sensor Performance Assessment (SPA) (A4) revised and now fully specified Product Quality Evaluation (A5) revised and now fully specified • Visualisation (A6) added • Calculate MMEs for PMD Data in Band Transfer Mode (AG.2) added • Check for Sunglint (AG.8) specified • Check for Rainbow (AG.9) specified • Error Calculations completely revised APPENDICES • Summary of Applicable Calibration Steps and Configurable Options (A) added • Coordinate Systems and Synchronisation (C) added • Instrument Calibration Considerations (E) revised • Measurement Uncertainty removed • Polarisation phase shift (E.4) revised • List of TBDs and TBCs (F) removed • Alphabetical Listing of References to GOME-2 PFS Variables (F) added
Issue 5: 1	31/5/2002	**EUM.EPS.SYS.DCR. 02.112**	CHAPTER 1 • Missing acronym definitions added CHAPTER 2 • Minor text modifications and clarifications CHAPTER 3 • Minor text modifications and clarifications CHAPTER 4 • Table 3 has been further revised with missing auxiliary sub-components added • Changes to requirements: ALG-HGH-060- added ALG-HGH-065- added ALG-HGH-070- added ALG-HGH-075- added ALG-HGH-080- added CHAPTER 5 • In Determine Observation Mode and Viewing Angles (A2.3) separation into individual earth modes added • Lunar geolocation further elaborated in Calculate Geolocation for Fixed Grid (A2.6). • Calculate Centre Coordinates (AG.19) added

Issue / Revision	Date	DCN. No	Changed Pages / Paragraphs
			• SAA lat/lon size reduced from 4 to 2. • Typographical errors removed. • A degradation correction factor dataset is now required at the beginning of in-orbit life of GOME-2 but will at this time contain default correction factors set to "one". Path length correction for the ozone line ratio corrected.
Issue 5: 2	14/6/2002	EUM.EPS.SYS.DCR. 02.127	CHAPTER 5 • Treatment of enumerated variables harmonised with PFS • Update of M-factors (degradation correction factors) now specified to be at the beginning of processing a product, not at the terminator • First page of section 5, type table: types character (c) and string (s) removed. Indicated 0=*false*, 1=*true* for boolean variables. • All boolean variables: Checked whether description matches usage and corrected description where needed. Determine PCDs from Geolocation: Formula for $N_{Sunglint}$ corrected in order to avoid counting high-risk scans twice. • Heading 5.3.19 corrected. • Determine UTC Time Grid: Note on MDR start/ stop time added. • Calculate Geolocation for Actual Integration Times: missing local variable T_f added to variable list. • Flag indicating LED status (derived from HK data) added to output of 'Calculate PPG'. • Dimension of pre-disperser prism temperature corrected • Figure 7b corrected to remove polarisation correction for *Sun* and *Moon* observation mode measurements • Note on incomplete integration times and band lengths added. • A2.0.1 Read Initialisation Data: Start/end pixels of valid data replaced by start/end wavelengths. • A2.0.1, A3.0.1 Read Initialisation Data: Default values filled in where missing. • A2.3.1 Determine Observation Mode: SLS/WLS currents/voltages must be valid for the SLS/WLS/SLS over diffuser modes: flags from previous step (A2.2 Convert HK data) are checked. • A2.7 Determine PCDs from geolocation: SAA check now uses satellite lat/lon instead of scan centre lat/lon because the latter is available only in earth observation modes. Sunglint and rainbow checks restricted to earth observation modes. New flag indicating possible mismatch between observation mode and geolocation. • AG.3 Convert HK Data: Logics for Lamp current/voltage check corrected. Valid range is now only checked if lamps are "on" (otherwise it would be invalid most of the time). Typos in SLS voltage check corrected. • AG.3 Convert HK Data: Extra equation given for integration time lookup. General: channel/band changed to either channel or band as appropriate.

Issue / Revision	Date	DCN. No	Changed Pages / Paragraphs
			• Appendix B: Treatment of incomplete PMD integration times and reporting of PMD integration times described. Layout of PMD arrays described. A2.1 Preprocess MMEs: Note on concatenation of main channel key data to single wavelength grid for PMDs added. Clarified that also key data errors are interpolated to common grid. Check of key data wavelength ranges against valid range from ini file added. • A2.16 Calculate Etalon Correction: Baseline correction (*LIN*) now calculated from linear fit instead of connecting start/end point. Several sums in the diagnostics changed from *ETS* to *ETE* instead of 0 to *D*–1. Residual set to zero outside the range (*ETS*, *ETE*). • Hot pixel mask, saturation mask: Dimension RFPA added as data granule is one scan. In AX.1, readout dimension *k* added to first equation in the algorithm section (creation of pixel mask). • More details provided for SPA. • Typographical errors corrected
Issue 5: 3	02/09/2002	EUM.EPS.SYS.DCR.02.155 Page and equation numbers (if any) relate to those from Issue 5:2 for easier tracking. Clarification GMV algorithm session 26 July 2002 MO-DCP-GMV-GO-0010 Clarification GMV algorithm session 26 July 2002 Clarification GMV algorithm session 29 July 2002 Clarification GMV algorithm session 29 July 2002 MO-DCP-GMV-GO-0009 Clarification GMV algorithm session 31 July 2002	A2.1.4 MME - Interpolation to fine grids: error condition required if extrapolation would be needed. A2.6.3 Calculate target pointing information - lunar mode: Normalisation was missing in eq. (96), corrected. A2.14 Calculate spectral calibration parameters for PMD channels: Missing index *n* / dimension BPMD added where needed A2.20 Calculate SMR: Variable table – Coordinate system for solar elevation specified A2.20.2 and first two of A2.20.3 were duplicate: corrected. A2.21.3 Calculate Stokes fractions: Clarified difference between marking individual Stokes fractions invalid and flagging the scan as containing invalid Stokes fractions. Treatment of reset pixels described in detail. Index typo corrected on p. 178. A3.10 Apply polarisation correction - Variable table: ⌈2 reference to PFS corrected A3.10 Apply polarisation correction: References to solar zenith angles and wavelength assignment removed (as this is performed already in A2.21 Determine Stokes fractions). A4.1.8 SPA - Preprocess Dark signal measurements: Missing band index j added in eq. (247) A4.2.1 SPA periodic time series analysis: Periodicity *T* added in eq. (249). AG15.2 Determine uniform straylight: Eq. (316) left side: index *i* removed (uniform straylight is not pixel dependent by definition!).

Issue / Revision	Date	DCN. No	Changed Pages / Paragraphs
		Clarification GMV algorithm session 31 July 2002 Clarification GMV algorithm session 26 July 2002 Clarification GMV algorithm session 31 July 2002 Clarification GMV algorithm session 31 July 2002	
Issue 5: 4	12/03/2004	EUM.EPS.SYS.DCR.04.006 Module and equation numbers refer to Issue 5:3	CHAPTER 1 • Document "history" updated to current status • Acronym list updated • [AD6] Note that preliminary coefficients are provided in Appendix F added • Issue information for [RD1], [RD2] and [RD3] removed CHAPTER 2 • Instrument characteristics updated to reflect current status CHAPTER 3 • Figures 3 and 4 and explanatory text updated to include externally provided time correlation data. • Entry added to Table 2 describing how missing external time correlation information is handled. CHAPTER 4 • Table 3 updated to include component 'Read Static Auxiliary Data (A2.0.3)' • Table 3 component 'Read Orbit Data (A2.0.2)' changed to 'Read Orbit and Time Correlation Data (A2.0.2)' • ALG-HGH-080 • ALG-FCT-030 • ALG-FCT-042 • ALG-FCT-044 • ALG-FCT-045 • ALG-INT-025 • ALG-INT-028 deleted *modified* *modified* added added
		DJO-SPR-GOME-92	CHAPTER 5 • A1.1.2 Standard CCITT 16-bit checksum replaced by a modified CCITT 16-bit checksum and the modification clarified

Issue / Revision	Date	DCN. No	Changed Pages / Paragraphs
		MO-DCP-GMV-GO-0011	• A2.1.1 Wavelength interpolation to MME grid: Clarification on number of pixels for PMD channels
		MO-DCP-GMV-GO-0012	A2.0.3 Read Key Data: Basic preprocessing of correction factor *C* for irradiance angular dependence added
			MO-DCP-GMV-GO-0013 • A2.0.1 Read Initialisation Data: Solar azimuth and elevation fine grid: Default values adapted to ranges covered by calibration key data. This affects variables *e*f, ∏f, N*ef*, and N∏f. MO-DCP-GMV-GO-0014 • A2.0.1 Read Initialisation Data: Nominal detector temperature range , for PMDs made the same as for main channels (230–240 K). MO-DCP-GMV-GO-0015 • A2.6 Calculate Geolocation for fixed grid: Latitude/ longitude for point F to be calculated at ground. MO-DCP-GMV-GO-0016 • A2.8.4 Calculate PCDs for dark signal correction: Clarification on eq. (119) added MO-DCP-GMV-GO-0018 • A2.20.2 Calculate SMR: Selection of readouts clarified MO-DCP-GMV-GO-0020 • AG.17.2 Interpolate MME describing irradiance response: Selection of angles clarified (take previous readout) MO-DCP-GMV-GO-0022 • A3.14 Reduce Spatial Aliasing: Specification clarified. MO-DCP-GMV-GO-0023 • A3.10.1 Establish Time Correlation between FPA and PMD channels: Index error corrected in eq. (214) (*i* replaced by *k*) MO-DCP-GMV-GO-0025 • A2.21 Determine Stokes fractions, A3.2 Calculate Geolocation for actual integration times, A3.10 Apply polarisation correction, A3.11 Apply radiance response, AG.17 Apply radiance response: Harmonised treatment of the situation where no previous scan exists (set corresponding output to “undefined”, set flag for degraded MDR). Suggestion to use negative infinity for internal representation of “undefined” output variables and reference to Generic PFS for their external representation added to introduction. MO-DCP-GMV-GO-0027 • AG.11 Normalise signals to one second IT: Note on PMD channels added (block dependent ITs have to be considered) MO-DCP-GMV-GO-0028 • A2.6.1 Determine sub-satellite point: Define *aocs* parameter (even if it is a dummy only) DJO-SPR-GOME-90 • A2.6.3 Calculate Target pointing information: Specification of R_{Earth} added. MO-DCP-GMV-GO-0029 • A2.20 Variable Table (p.166): references to irradiance response correction removed. (Although formally correct, they led to confusion.) MO-DCP-GMV-GO-0030 • AG.17 Apply Irradiance Response: Coordinate System (Satellite Relative Actual Reference CS) specified in variable table. Sign for solar elevation corrected by replacing reference to eq. (340) by eq. (338) which is the one to use for the Satellite

Issue / Revision	Date	DCN. No	Changed Pages / Paragraphs
			Relative Actual Reference CS. MO-DCP-GMV-GO-0031 MOtimes: 1. Condition covering backscan from previous
			GPP phase 3 change • A2.21 Determine Stokes fractions: Single-scattering Stokes fraction *u* and polarisation angle ⎜ calculated. Bad Stokes fractions flag added to PCD, and Bad Stokes fractions counter to global counters (for SPHR). “Invalid” Stokes fractions renamed to “missing” and product reference corrected from PCD_BASIC to PCD_EARTH. References to product fields updated to take into account corresponding changes in PFS (affected compounds: POLSS and POLV). Measure for scene inhomogeneity added. Errors on Stokes fractions, stored in POL_M(_P) Q_POL_ERR, clarified to be set to “undefined” GPP phase 3 change • A2.21 Determine Stokes fractions, A3.10 Apply polarisation correction: Last two dimensions of interchanged for consistency with PFS. GPP phase 3 change • A3.0 Read input data: References to specific GEADRs added GPP phase 3 change • A3.0.2 Read static auxiliary dataset, A3.15 Calculate fractional cloud cover and cloud top pressure: Units for surface elevation corrected from km to m GPP phase 3 change • A3.2 Calculate Geolocation for actual integration times: Scanner viewing angles added. Solar and satellite zenith and azimuth angles added. Integration time 93.75 ms without co-adding treated separately. GPP phase 3 change • A3.10 Apply polarisation correction: MME ⌠3 and Stokes component *u* added. Updated references to product fields to take into account corresponding changes in PFS (affected compounds: POLSS and POLV). GPP phase 3 change • A3.11 Apply radiance response: PMD channels are combined into a single PMD radiance. Array dimensions and indices added to account for readout dimension within scan. GPP phase 3 change • A3.15 & A3.0.2 Calculate Fractional Cloud Cover and Cloud Top Pressure & Read Static Auxiliary Data: Land/Sea Mask removed. measurements over sea are now treated in the same manner as those over land. Addition output parameters written to level 1b product. GPP phase 3 change • A3.17.3: Generate Header and Global Product Information: Source of band start/end wavelengths added GPP phase 3 change • A4.2.13 Monitor instrument throughput using solar measurements: typo in equation corrected (*t* replaced by ⎣)
			GPP phase 3 change • AG.2 Calculate MMEs for PMD data in band transfer mode: MME ⌠3 added Correction • AG.2 Index typo corrected in equations (263) to (266) GPP phase 3 change • AG.8 Check for sunglint: land-sea mask introduced and sunglint checked over water only. GPP phase 3 change • AG.17: Missing reference to AG.2 inserted in “Use generic sub-functions” GPP phase 3 change APPENDIX • Appendix A: Change in applicability of steps in 1a processing for WLS mode. GPP phase 3 change • Appendix F containing preliminary HK data conversion coefficients inserted (Alphabetical Listing of References to GOME-2 PFS Variables becomes Appendix G)

Issue / Revision	Date	DCN. No	Changed Pages / Paragraphs
Issue 6: 0	19/03/2004	EUM.EPS.SYS.DCR.04.023 Module and equation numbers refer to Issue 5:4	CHAPTER 1 • Document "history" updated to current status
Issue 6: 1	9/03/2006	EUM.SYS.DCR.06.0307 MO-DCP-ESA-GO-004 & MO-DCP-ESA-GO-025 MO-DCP-ESA-GO-011 & MO-DCP-ESA-GO-017 & MO-DCP-ESA-GO-018 & MO-DCP-ESA-GO-020 & MO-DCP-ESA-GO-024 EUM.EPS.NCR.1229 & MO-DCP-ESA-GO-005 MO-DCP-ESA-GO-019 MO-DCP-ESA-GO-023 EUM.EPS.AR.1831 & MO-DCP-ESA-GO-007 & MO-DCP-ESA-GO-022 MO-DCP-ESA-GO-015 & MO-DCP-ESA-GO-021 EUM.EPS.AR.1828 & MO-DCP-ESA-GO-009 MO-DCP-ESA-GO-016 MO-DCP-ESA-GO-013 & MO-DCP-ESA-GO-027 MO-DCP-ESA-GO-010 & MO-DCP-ESA-GO-014 MO-DCP-ESA-GO-012	CHAPTER 5 • Change data types from float to double everywhere to be consistent with both the PPF and GPP implementations including reference to C maths library. • A2.0 Read Initialisation Data: Change indications provided for default MME viewing angle grid to be consistent with Key data. Threshold values for old IFC data added. Switch for PPG backup light source added. Parameters for spatial aliasing wavelength extrapolation added. FPA wavelength calibration initialisation parameters modified. Parameter for SLS low voltage mode added. • A2.1 Preprocess Müller Matrix Elements: Use average of BSDF_CU_S and BSDF_CU_P for epsilon BSDF to resolve ambiguity. • A2.3.2 Determine UTC Time Grid: Revised to take account of the SBT counter rollover on the basis of information provided by DJO at FAT. • A2.8 Calculate Dark Signal: Allow channel dependent offset for PCD calculation. • A2.13 Calculate Spectral Calibration Parameters for Main Channels: Use absolute values of deviations to calculate max and mean deviations. Indicate Key data file to be used in case of SLS low voltage mode. • A2.14 Calculate Spectral Calibration Parameters for PMD Channels: Interpolation of SLS Stokes fractions to FPA grid added. Algorithm consolidated on the basis of input from the PPF and GPP alignment process. Revise definition of equidistant grid and related initialisation parameters. • A2.16 Calculate Etalon Correction: Minor clarifications and corrections to improve numerical performance. • A2.20 Calculate SMR: Editorial correction. • A3.10 Apply Polarisation Correction: Minor corrections and improvements added on the basis of input from the PPF and GPP alignment process. • AG.8 Check for Sunglint: Correct relative azimuth angle and replace "line-of-sight" angles with "satellite" angles for consistent terminology. • AG.17 Apply Irradiance Response: Clarify timestamping of PMD readouts in raw transfer mode.
v.7	28 Feb 2011	MO-DCP-ESA-GO-026	APPENDIX B • Correct description of PMD solar readout mode.
v.8	8 August 2014	EUM/AdminTools/AR/144.1	Document transcribed from Framemaker to Word DocX version. No changes to text. New published document is version 8. Document reviewed for publication. Only changes to signature list.

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1 INTRODUCTION

1.1 Purpose and Scope of Document

This Product Generation Specification (PGS) specifies the requirements for the Metop GOME-2 instrument Level 1 Product Generation Function (PGF).This document has initially been prepared on the basis of input received from DLR-MF as part of the GOME-2 Ground Processor Prototype (GPP) Phase B study. The input from DLR-MF was prepared by S. Slijkhuis and W. Balzer with further input from A. von Bargen, E. Hegels. Algo-rithms related to polarisation measurements and polarisation correction have been provided by I.Aben, W. Hartmann, and C. Tanzi of SRON. Furthermore the FRESCO algorithm [RD20] for determination of cloud top pressure and effective cloud fraction was generously provided by P.Stammes and N. Fournier of KNMI and R. Koelemeijer formerly of KNMI. During the phase C/D (implementation) of the GOME-2 GPP valuable feedback was provided by GMV (project managers L. M. González Casillas and C. Gomez Cid). This feedback was implemented into this document in form of corrections and clarifications. In parallel, detailed results from the on-ground calibration of the GOME-2 instrument have become available. Some of them necessitated adaptations of algorithms or interfaces to calibration keydata. Section 1 of this document is this introduction.

1.2 Structure of the Document

The document is organised in the following sections:

Section 1	of this document is this Introduction.
Section 2	gives background information on the GOME-2 instrument properties and instrument operation.
Section 3	of this document provides a short overview of the overall concept of the PGF as a component in a larger system. It also describes the way in which the PGF is expected to be operated.
Section 4	contains the requirements on the PGF.
Section 5	contains the scientific and mathematical algorithm specifications that support the requirements.

1.3 Document Evolution

This document has evolved in response to further information made available to EUMETSAT from alignment of the GOME-2 operational processor and the ground processor prototype after the release of Issue 6 Revision 0. Detailed changes between Issue 6 Revision 0 and Issue 6 Revision 1 are described in the Document Change Record at the beginning of this document.

1.4 Acronyms Used in this Document

Acronym	Meaning
ADC	Analog to Digital Converter
ATBD	Algorithm Theoretical Basis Document
BISA	Belgium Institute for Space Aeronomy (Brussels/Uccle, B)
BSDF	Bi-directional Scattering Distribution Function
BU	Binary Unit
CAL	Calibration function of EPS
CFI	Customer Furnished Item
CGS	Core Ground Segment
CGSRD	Core Ground Segment Requirements Document
CS	CS Coordinate System
CU	Calibration Unit of the GOME 2 instrument
DLR	Deutsches Zentrum für Luft und Raumfahrt e.V.
DLR	MF Institut für Methodik der Fernerkundung, DLR (Oberpfaffenhofen, D)
DOAS	Differential Optical Absorption Spectroscopy
DSM	Default Settings Mode
EPS	Eumetsat Polar System
EQM	Engineering Qualification Model
ERS	European Remote Sensing Satellite
ESA	European Space Agency
ESTEC	European Space Technology Centre (Noordwijk NL)
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FM	Flight Model. GOME-2 has three flight models: labelled FM1, FM2, FM3.
FOV	Field of View
FPA	Focal Plane Assembly (used in this document to denote GOME-2 main channels: FPA 1-4 in contrast to PMD channels)
FWHM	Full Width at Half Maximum
GDP	(ERS-2) GOME Data Processor
GEADR	Global External Auxiliary Data Record
GIADR	Global Internal Auxiliary Data Record
GMV	Grupo de Mechánica del Vuelo
GOME	Global Ozone Monitoring Experiment
GPP	Ground Processor Prototype
HCL	Hollow Cathode Lamp
HK	Housekeeping
HMI	Human Machine Interface
IFE	Institut für Fernerkundung der Universität Bremen (D)
IFOV	Instantaneous Field of View
ILOS	Instantaneous Line of Sight
ISAO-CNR	Institute of Atmospheric and Oceanic Sciences (Bologna, I)
IT	Integration Time

Acronym	*Meaning*
KNMI	Koninklijk Nederlands Meteorologisch Instituut (De Bilt, NL)
LED	Light Emitting Diode
LOS	Line of Sight
MCS	Mission Control System
MetOp	Meteorological Operational Satellite
MJD	Modified Julian Date
MME	Müller Matrix Element
MPHR	Main Product Header Record
NRT	Near Real Time
PCD	Product Confidence Data
PGE	Product Generation Environment of EPS
PGF	Product Generation Function of EPS
PMD	Polarisation Measurement Device
PPG	Pixel-to-Pixel Gain Pixel-to-Pixel Gain
PQE	Product Quality Evaluation
QCS	Quality Control Support function of EPS
QA	Quality Assessment
QTH	Quartz Tungsten Halogen
RAL	Rutherford Appleton Laboratory (Oxford, UK)
SAA	Southern Atlantic Anomaly
SAO	Smithsonian Astrophysical Observatory (Cambridge, USA
SPA	Sensor Performance Assessment
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Cartography
SLS	Spectral Light Source
SMR	Sun Mean Reference
SRON	Space Research Organisation of The Netherlands (Utrecht, NL)
SVD	Singular Value Decomposition
SZA	Solar Zenith Angle
TOA	Top of Atmosphere
TPD	Technisch Physische Dienst (Delft, NL)
UTC	Universal Time Co-ordinate
UV	Ultra-Violet
VIADR	Variable Internal Auxiliary Data Record
VIS	Visible
WLS	White Light Source

1.5 Definitions

For the definitions used in this document, including the reference frames to be used, see the Mission Conventions Document (MCD) [AD7], and the Product Conventions Document (PCD) [AD8].

1.6 Applicable and Reference Documents

The instrument Product Generation Function (PGF) is a constituent of the CGS. Therefore, unless otherwise specified, all the requirements of the Core Ground Segment Requirements Document (CGSRD) [AD1] apply to this Product Generation Function. In particular, the instrument Product Generation Function shall comply with all the requirements on the generic PGE services.

In case of conflict between these Product Generation Function requirements and Core Ground Segment Requirements Document (CGSRD) [AD1] requirements, the latter shall take precedence.

1.7 Applicable Documents

	Document Name	*Reference*
AD 1	EPS Core Ground Segment Requirements Documents	EPS/GGS/REQ/95327
AD 2	EPS CGS to Product Generation Function IRD	EPS/GGS/IRD/980255
AD 3	EPS Product Convention Document	EPS/SYS/TEN/990007
AD 4	EPS Generic Product Format Specification	EPS/GGS/SPE/96167
AD 5	GOME-2 Level 1 Product Format Specification	EPS/MIS/SPE/97232
AD 6	GOME-2 Instrument TM/TC list Preliminary Coefficients for use in processor testing are specified in Appendix F of this document.	
AD 7	EPS Mission Conventions Document	EPS/GGS/SPE/990002
AD 8	Product Convention Document	EPS/SYS/TEN/990007
AD 9	GOME-2 Science Data Packet Definition	MO-DS-LAB-GO-0006
AD 10	GOME-2 Command Word Definition	MO-DS-LAB-GO-0005

1.8 Reference Documents

	Document Name	*Reference Number*
RD 1	GOME-2 Requirements Specification	MO-RS-ESA-GO-0071
RD 2	GOME-2 Calibration Plan	MO-PL-TPD-GO-0004
RD 3	GOME-2 Calibration Error Budget	MO-RS-TPD-GO-0016
RD 4	MetOp Mission CFI Software	Description and Interface Definition Document, MOTN-ESA-CF-0140, Issue Draft, 23 Apr 1999
RD 5	MetOp Mission CFI Conventions Document	MO-TN-ESA-ST-0194, Issue Draft, 16 Aug 1999
RD 6	Hiroshi Akima, "A new method of interpolation and smooth curve fitting based on local procedures"	J. ACM, Vol. 17(4), 1970, 589-602
RD 7	Data Reduction from Experimental Histograms, W.R. Falk (University of Manitoba, Winnipeg, Canada),	Nuclear Instruments and Methods in Physics Research 220 (1984) 473-478
RD 8	John Tonry and Marc Davis, “A survey of galaxy redshifts. 1. Data reduction techniques”,	Astron. J.,Vol. 84(10), 1979, 1511-1525

	Document Name	*Reference Number*
RD 9	William H. Press et al., “Numerical Recipes in C”	Cambridge University Press, 1994
RD 10	William H. Press et al., “Numerical Recipes in Fortran - The Art of Scientific Computing - Second Edition”,	Cambridge University Press, 1992.
RD 11	Jochen Stutz and Ulrich Platt, "Problems in using diode arrays for open path DOAS measurements of atmospheric species",	Institut für Umweltphysik, Universität Heidelberg.
RD 12	Piet Stammes, "The seventh point polarisation algorithm, Internal Report" (GOME and SCIAMACHY),	KNMI De Bilt, 1994
RD 13	P. Stammes, I. Aben, R.B.A. Koelemeijer, S. Slijkhuis, D.M. Stam, "GOME polarisation validation study", Proceedings of the Third ERS Symposium on "Space at the Service of our Environment",	ESA SP-414, Vol. II, 669-674, Florence 1997
RD 14	N. Schutgens, KNMI, private communication, December 1999	
RD 15	P. Stammes, I. Aben, R.B.A. Koelemeijer, S. Slijkhuis, R. Spurr, D.M. Stam, "Polarisation correction of GOME measurements of the Earth’s radiance spectrum”	in preparation, 2000
RD 16	R.J. Woodham and M.H. Gray, "An Analytic Method for Radiometric Correction of Satellite Multispectral Scanner Data", IEEE Transactions on Geoscience and Remote Sensing,	Vol. GE-25 (3), May 1987
RD 17	B. Jaehne, "Digital Image Processing"	Springer-Verlage 1997
RD 18	D. Loyola, "A New Cloud Recognition Algorithm for Optical Sensors",	IEEE – Proceedings of ISAMS conference, Seattle, 1998
RD 19	E. Matthews, “Vegetation, land-use, and albedo data sets",	Technical Memo 86107, NASA, May 1984.
RD 20	R.B.A, Koelemeijer, P. Stammes, J.W. Hovenier and J.F. de Haan, “A fast method for retrieval of cloud parameters using oxygen A-Band measurements from GOME”, JGR,	Vol 106, 3475-3490, 2001.
RD 21	R.B.A, Koelemeijer, P. Stammes, J.W. Hovenier and J.F. de Haan, “Global distributions of effective cloud fraction and cloud top pressure derived from oxygen A-band spectra measured by GOME: comparison to ISCCP data”	JGR, *in press*, 2002.

1.9 Background Information on the GOME/ SCIMACHY Family of Sensors

	Document Name	*Reference Number*
BD 1	Burrows, J. P., K. Chance, P. Crutzen, H. van Dop, J. Geary, T. Johnson, G. Harris, I Isaksen, G. Moortgat, C. Muller, D. Perner, U. Platt, J. -P. Pommereau, H. Rodhe, E. Roeckner, W. Schneider, P. Simon, H. Sundquist, and J. Vercheval, SCIAMACHY A European proposal for atmospheric remote sensing from the ESA polar platform,	Max- Planck Institut fur Chemie, Mainz, Germany, 1988
BD 2	Burrows J.P., Chance K.V., "SCIAMACHY and GOME: the scientific objectives"	Optical Methods in Atmospheric Chemistry, SPIE Vol. 1715, 1992
BD 3	GOME Geophysical Validation Campaign, Final results Workshop Proceedings,	ESA WPP-108, May 1996
BD 4	OMI - Ozone Monitoring Instrument for MetOp, Report of the OMI User Advisory Group,	ESA WPP-123, October 1996, and references therein
BD 5	ESAMS'99 - European Symposium on Atmospheric Measurements from Space	ESA WPP-161, Vol. I&II, ISSN 1022-6656, March 1999

1.10 ERS-2/GOME and SCIAMACHY Project Documentation and Reports

	Document Name	*Reference Number*
GD 1	GOME Interim Science Report, by Burrows J. P., K. V. Chance, A. P. H. Goede, R. Guzzi, B. J. Kerridge, C. Muller, D. Perner, U. Platt, J.-P. Pommereau, W. Schneider, R. J. Spurr, H. van der Woerd, edited by T. D. Guyenne and C. J. Readings	SP-1151 ESA publications Division, ESTEC, Noordwijk, The Netherlands, ISBN 92-9092-041-6 (1993)
GD 2	GOME Users Manual,	ESA SP-1182, ESA/ESTEC, Noordwijk, The Netherlands (1996)
GD 3	GOME Level 0 to 1b Algorithm Description, ER-TN-DLR-GO-0022, Issue 4/A, August 1996.	ER-TN-DLR-GO-0022, Issue 4/A, August 1996.
GD 4	GOME Data Processor - Extraction Software User's Manual,	ER-SUM-DLR-GO-0045, Issue 1, 4.8.1999
GD 5	GOME Data Processor - Update Report for GDP 0-to-1 Version 2.0 and GDP 1-to-2 Version	ER-TN-DLR-GO-0043, Issue 1/A, 24.8.1999
GD 6	GOME Data Quality Improvement (GDAQI) - Final Report,	TN-GDAQI-003SR/2000, September 29, 2000
GD 7	SCIAMACHY Level 0 to 1c Processing - Algorithm Theoretical Basis Document, ENVATB-	DLR-SCIA-0041, Issue 1, 19.2.1999

2 OVERVIEW OF THE GOME-2 INSTRUMENT

2.1 Background Information

Detailed requirements for the level 0 to 1b processing are laid down in Chapter 4, which amongst other things takes account of the GOME-2 requirements for calibration [RD1] and the GOME-2 Calibration Plan [RD2] (based on the instrument design), and of the requirements imposed by the generic environment for all MetOp ground processors [AD1], by the level 0 data availability [AD9], [AD10], and by the data product definition [AD4], [AD5] and requirements:

2.2 Relation to GOME on ERS-2

The Global Ozone Monitoring Experiment (GOME) was originally conceived as a scaled-down version of SCIAMACHY. It was given fast-track development status by ESA [GD1], and was launched on 21 April 1995 on board the second European Remote Sensing Satellite (ERS-2). GOME is a nadir scanning spectrometer covering the spectral range 240–790 nm. The measurement capability of GOME closely matches the UV/visible nadir capability of SCIAMACHY which in addition has limb viewing capability and a wavelength range extended into the near infrared. The mission objectives [BD1], [BD2] of GOME and SCIAMACHY are very similar.

The GOME Data Processor (GDP) [GD2] was developed and implemented at DLR, Oberpfaffenhofen, Germany, with scientific support of several institutions, notably the University of Heidelberg, the University of Bremen (IFE), SAO, KNMI, ISAO-CNR, RAL, and the Max Planck Institute for Chemistry. The GDP became operational in July 1996, with calibrated earthshine spectra and total ozone columns being the main products generated on a routine basis. Since then the GDP has been further developed by DLR taking inputs from SRON, BISA, and several of the above institutions [GD5], [GD6].

The GOME-2 instrument was selected in part as a result of the experience accumulated during a number of years of operations and data analysis from GOME on ERS-2. The large range of products which have been obtained from GOME data has clearly demonstrated the capability of this class of instrument to contribute to the operational meteorology and climate monitoring objectives of the EPS mission. Furthermore, the in-flight performance of GOME and its reliability has proven its suitability for use as an operational instrument. Although the basic design of GOME-2 is the same as that of GOME, a number of technical improvements have been made both in response to knowledge gained from GOME operations on ERS-2, and also in response to increasingly-stringent user requirements. Changes which will provide enhanced performance of GOME-2 as compared to ERS-2 GOME include the following [8]:

- Improved polarisation measuring capability
- Inclusion of a new on-board white light source
- Increased maximum swath width
- Integration time reduced to provide smaller ground pixels
- Increased spectral sampling to minimise undersampling effects
- Higher data rate
- Quartz quasi-volume diffuser to reduce spectral artifacts in irradiance measurements.

2.3 Gome-2 Instrument Characteristics and Operating Modes

2.3.1 Instrument Hardware

GOME-2 is a medium-resolution UV-VIS spectrometer, fed by a scan mirror which enables across-track scanning in nadir, as well as sideways viewing for polar coverage and instrument characterisation measurements using the moon. This scan mirror can also be directed towards internal calibration sources or towards a diffuser plate for calibration measurements using the sun.

GOME-2 comprises four main optical channels which focus the spectrum on linear detector arrays of 1024 pixels each, and two Polarisation Measurement Devices (PMDs) containing the same type of arrays for measurement of linearly polarised intensity in two perpendicular directions. Compared to the main channels, the PMD measurements are performed at lower spectral resolution, but at higher spatial resolution which facilitates sub-pixel determination of cloud coverage. The PMDs are required because GOME-2 is a polarisation sensitive instrument. Therefore, the intensity calibration of GOME-2 has to take account of the polarisation state of the incoming light using information from the PMDs.

The four main channels provide continuous spectral coverage of the wavelengths between 240 nm and 790 nm with a spectral resolution (FWHM) between 0.26 nm and 0.51 nm. Channel characteristics are listed in Table 1.

Channel	*Spectral Range (nm)*	*Detector Pixel Size (nm)*	*FWHM (nm)*
1	240 – 314	0.12	0.26
2	310 – 403	0.12	0.27
3	397 – 604	0.21	0.51
4	593 – 790	0.21	0.48
PMD p PMD s	312 – 790	0.62 (312 nm) – 8.8 (790 nm)	2.9 (312 nm) – 37 (790 nm)

Table 1: GOME-2 spectral coverage and resolution. Values are given for GOME-2 FM3. For the overlap regions between the main channels, the wavelengths are given for the 10% intensity points. E.g., at 310 nm, 10% of the signal is registered in channel 2, and 90% in channel 1. At 314 nm, 10% of the signal is registered in channel 1, and 90% in channel 2. Spectral resolution (FWHM) varies slightly across each main channel, the given values are channel averages.

The optical configuration of the instrument is shown in Figure 1. Light enters the two-mirror telescope system via the scan mirror. The telescope projects the light beam onto the slit which determines the instantaneous field-of-view (IFOV) of 0.28° × 2.8° (across track × along track). After it has passed the slit, the beam is collimated again and enters a double Brewster prism for partial split-off to PMD s, followed by the pre-disperser prism which has two functions. Brewster reflection at the back of the prism splits off part of the p-polarisation direction to PMD p. The prism furthermore forms a low-dispersion spectrum which is subsequently separated at the channel separator prism into three parts going to channels 1 (transmitted beam), 2 (reflected beam), and 3 and 4, respectively. The separation between channels 3 and 4 is performed by a dichroic filter. A grating in each channel then further disperses the light which is subsequently focused onto the detector array. Each PMD channel contains a dispersion prism and two additional folding prisms and collimating lenses. PMD p measures intensity polarised parallel to the spectrometer’s slit, and PMD s measures intensity polarised perpendicular to the spectrometer’s slit. The two PMD channels are designed in a way that maximum similarity in their optical properties is ensured. The wavelength-dependent dispersion of the prisms causes a much higher spectral resolution in the ultraviolet than in the red part of the spectrum.

To reduce the dark signal, the detectors of the main channels are actively cooled to temperatures around 235 K by Peltier elements in a closed control loop. The PMDs are cooled by Peltier elements in an open loop configuration and will have detector temperatures around 235 K (the actual value will depend on in-orbit instrument temperature and PMD cooler settings). The optical bench is not cooled, and its operational temperature is expected to be between 268 K and 288 K.

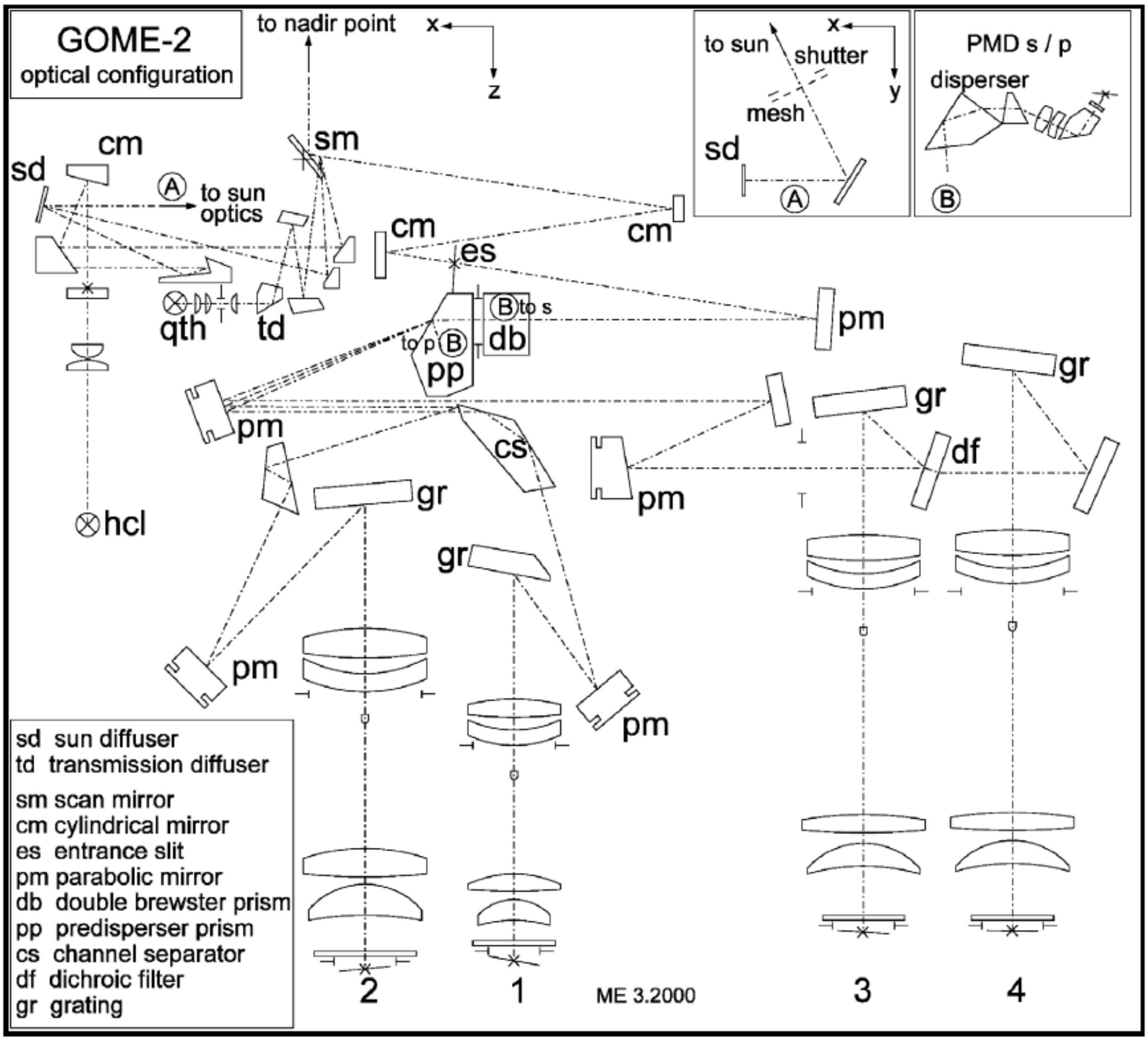

Figure 1: GOME-2 optical layout. The optics lie in one plane (except insets A and B). Nadir is in − Z direction, the flight direction is − Y; X is towards 'East'.

To calculate the transmission of the atmosphere, which contains the relevant information on trace gas concentration, the solar radiation incident on the atmosphere must be known. For this measurement a solar viewing port is located on the flight-direction side of the instrument. When this port is opened, sunlight is directed via a ~40° incidence mirror to a diffuser plate. Light scattered from this plate, or in general, light from other calibration sources such as the Spectral Light Source (SLS) for wavelength calibration, and the White Light Source (WLS) for etalon (and, optionally, pixel-to-pixel gain) calibration are directed to the scan mirror using auxiliary optics. Diffuser reflectivity can be monitored internally using light from the SLS. All internal calibration sources with their optics are assembled in a subsystem called the 'Calibration Unit' (CU). The only exception is light-emitting diodes (LEDs) which are located in front of the detectors to monitor the pixel-to-pixel gain.

2.3.2 Data Packet Structure and Basic Instrument Operation

GOME-2 generates one science data packet every 375 milliseconds. A data packet comprises 9369 two-byte words, leading to an average data rate of (8 × 2) × 9369/0.375 bit/s = 400 kbit/s or 300 MB/orbit. A detailed description of the science data packet format is provided in [AD9]. Briefly, a GOME-2 data packet consists (apart from header information) of three parts: instrument housekeeping (HK) data (temperatures, scan mirror angles, lamp currents and voltages), PMD data and main channel FPA data. The maximum temporal resolution differs between main channel. FPA and PMD data. One data packet contains up to 2 main FPA readouts, corresponding to a 187.5 ms temporal resolution, and up to 16 PMD readouts, corresponding to a 23.4 ms temporal resolution. A detailed description of the options for PMD readout and data transfer is given in Appendix B.

A basic concept in the operation of the GOME-2 instrument is that of the '**scan**'. A scan is defined as a time interval of 6 seconds, consisting of 16 **'subsets'** of 375ms each. The subsets are numbered from 0 to 15. In the earth scanning mode, a scan consists of one scan cycle: 4.5 seconds forward scan (subsets 0 to 11) and 1.5s flyback (subsets 12 to 15, see Figure 2). In the static and calibration modes the scan mirror does not move, but the data packet structure is identical with the scanning mode.

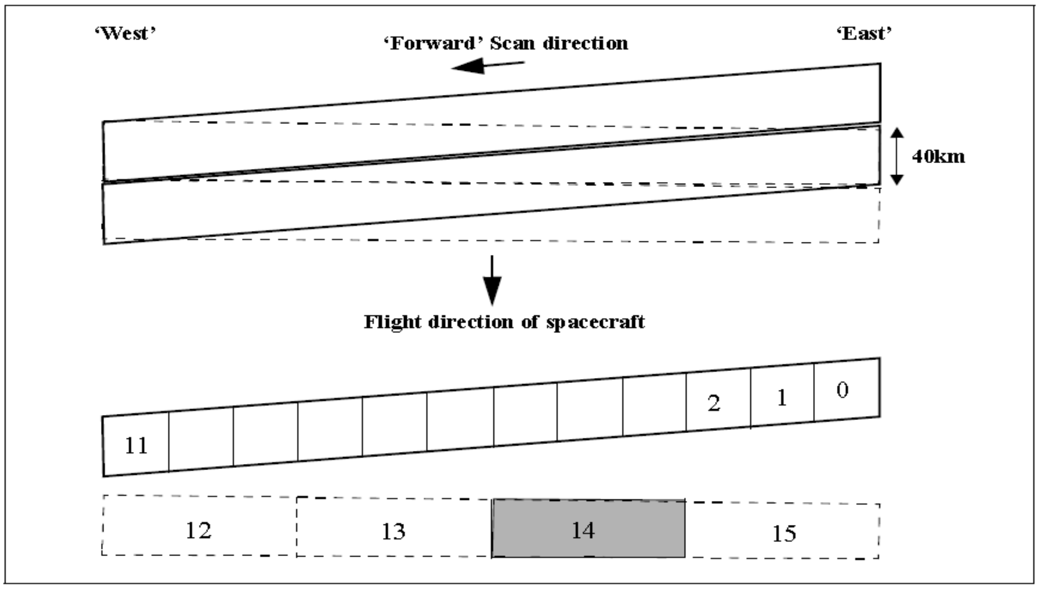

Figure 2: Scan pattern in default scan mode. Solid line: forward scan; dashed line: flyback. Each subset pixel (0–15) corresponds to 375 milliseconds. In one of the four subsets of the flyback (subset 14 is shown as an example only) the 'unused' parts of the PMD detectors (Block A see Appendix B) are read out.

In the default measuring mode, the nadir scan, the scan mirror sweeps in 4.5 seconds (12 subsets) from negative to positive viewing angles, followed by a flyback of 1.5 seconds (the last 4 subsets) back to negative viewing angles. The default swath width of the scan is 1920 km which enables global coverage of the Earth's surface within 1.5 days. Other swath widths (960, 320, 240, and 120 km) and the swath centre can be commanded. The scan mirror speed can be adjusted such that, despite the projection effect, the ground is scanned at constant speed. The along-track dimension of the instantaneous field-of-view (IFOV) is ~40 km which is matched with the spacecraft velocity, such that each scan closely follows the ground coverage of the previous one. The IFOV across-track dimension is ~4 km. For the 1920 km swath, the maximum temporal resolution of 187.5 ms for the main channels (23.4 ms for the PMD channels) corresponds to a maximum ground pixel resolution (across track × along track, Figure 2) of 80 km × 40 km (10 km × 40 km for the PMDs) in the forward scan.

The actual integration time used (and thus the ground pixel size) will depend on the light intensity. The integration time can be separately set for each channel; in channel 1 and 2 it is even possible to subdivide the channel in two parts (called 'band 1a', 'band 1b' and 'band 2a', 'band 2b' respectively) having separate integration times. It is anticipated that a default integration time of 187.5 ms (yielding two spectrum readouts per data packet) will be used in all channels with two exceptions where longer integration times are needed because of low light intensity:

(i) Band 1a has a default integration time of 1.5 seconds (yielding one spectrum every second scan).

(ii) The integration time for all channels will be increased for low solar elevations (high solar zenith angles).

2.3.3 Summary of Observation Modes

This section gives a classification of the GOME-2 observation modes. The observation modes can be assigned to three categories: earth observation modes, calibration modes, and other modes.

The data processor has to derive the observation mode by combining fields from the data packet, such as scan mirror position, subsystem status flags, etc. There is no dedicated field in the data packet indicating the observation mode. Any GOME-2 data packet which does not fit into one of the modes below will be classified as "invalid" by the data processor. The observation mode will be determined in processor module A2.3.

2.3.3.1 Earth observation modes

Earth observation (or "earthshine") modes are those modes where the earth is in the field of view of GOME-2. They are usually employed on the dayside of the earth (sunlit part of the orbit). The scan mirror can be at a fixed position (static modes), or scanning around a certain position (scanning modes). All internal light sources are switched off and the solar port of the calibration unit is closed.

NADIR SCANNING	This is the mode in which GOME-2 will be operated most of the time. The scan mirror performs a nadir swath as described above. The swath width is commandable, its default value is 1920 km. Scanning can be performed either with constant ground speed, resulting in equally sized ground pixels (this is the default), or with constant angular speed ("GOME-1 mode"), resulting in larger ground pixels for the extreme swath positions as compared to the swath centre.
NORTH POLAR SCANNING	The scan mirror performs a (narrow) swath around the viewing angle +46.696º (default value) in order to cover the North Polar region with a high spatial resolution. This mode will typically be used during Northern hemisphere spring.
SOUTH POLAR SCANNING	The scan mirror performs a (narrow) swath around the viewing angle – 46.172º (default value) in order to cover the South Polar region with a high spatial resolution. This mode will typically be used during Southern hemisphere spring.
OTHER SCANNING	The scan mirror performs a swath around another off-nadir position.
NADIR STATIC	The scan mirror is pointing towards nadir. This mode will typically be used during the monthly calibration. It is valuable for validation and long-loop sensor performance monitoring purposes.
OTHER STATIC	The scan mirror is pointing towards an off-nadir position.

2.3.3.2 Calibration Modes

In-orbit instrument calibration and characterisation data are acquired in the various calibration modes. They are usually employed during eclipse with the exception of the solar calibration which is performed at sunrise. Both internal (WLS, SLS, LED) and external (sun, moon) light sources can be employed. The various sources are selected by the scan mirror position.

Dark	The scan mirror points towards the GOME-2 telescope. All internal light sources are switched off and the solar port is closed. Dark signals are typically measured every orbit during eclipse.
Sun (Over Diffuser)	The scan mirror points towards the diffuser. All internal light sources are switched off and the solar port is open. Solar spectra are typically acquired once per day at the terminator in the Northern hemisphere. The Sun Mean Reference (SMR) spectrum will be derived from this mode.
White Light Source (Direct)	The scan mirror points towards the WLS output mirror. The WLS is switched on and the solar port is closed. The WLS can be operated at four different currents: 360 mA, 380 mA, 400 mA, and 420 mA). Etalon (and optionally PPG) calibration data will be derived from this mode.
Spectral Light Source (Direct)	The scan mirror points towards the SLS output mirror. The SLS is switched on and the solar port is closed. Wavelength calibration coefficients will be derived from this mode.

Spectral Light Source Over Diffuser	The scan mirror points towards the diffuser. The SLS is switched on and the solar port is closed. Light from the SLS reaches the scan mirror via the diffuser. This mode is employed for in-orbit monitoring of the sun diffuser reflectivity.
Led	The scan mirror points towards the GOME-2 telescope. The LEDs are switched on and the solar port is closed. PPG calibration data will be derived from this mode.
Moon	The scan mirror points towards the moon (typical viewing angles are + 70º to + 85º). As the spacecraft moves along the orbit, the moon passes the GOME-2 slit within a few minutes. This mode can be employed only if geometrical conditions (lunar azimuth, elevation and pass angle) allow it which will typically occur a few times per year. It is employed as an additional mode for in-orbit performance monitoring.

2.3.3.3 Other modes

These modes are either transitory (idle mode) or used in instrument maintenance (dump and test modes). In these modes, data packets are generated; however, they do not contain any useful scientific data.

Idle	This mode is reached during instrument switch-on or switch-off.
Dump	In place of PMD and main channel data, memory contents are down linked. This mode is used for diagnostic purposes.
Test	In place of PMD and main channel data, a fixed test pattern is down linked. This mode is used for diagnostic purposes.

3 SYSTEM AND OPERATIONS CONCEPT

3.1 System Concept

3.1.1 System Context

The Product Generation Function is a constituent function of the Core Ground Segment. In particular, the Core Ground Segment contains the Product Generation Environment (PGE), which provides the interface between the CGS and PGF. Please see the CGSRD [AD1] for details of the PGE.

For the purposes of this discussion, it is sufficient to identify that the PGE relationship with the PGF provides:

- a library of functions,
- data input and output interfaces,
- commanding of the PGF,
- infrastructure for PGF operations.

This context is mentioned in order to reinforce the concept that the PGF is a constituent function of the Core Ground Segment and so this PGF should be read in conjunction with the Core Ground Segment documentation. The primary objective of the EPS ground segment is to process data received from NOAA and MetOp satellites and distribute this data to Eumetsat member states. A more detailed description of the various functions of the Core Ground Segment is given in [AD1].

3.1.2 Context of the Product Generation Function (A0)

3.1.2.1 Major Interfaces

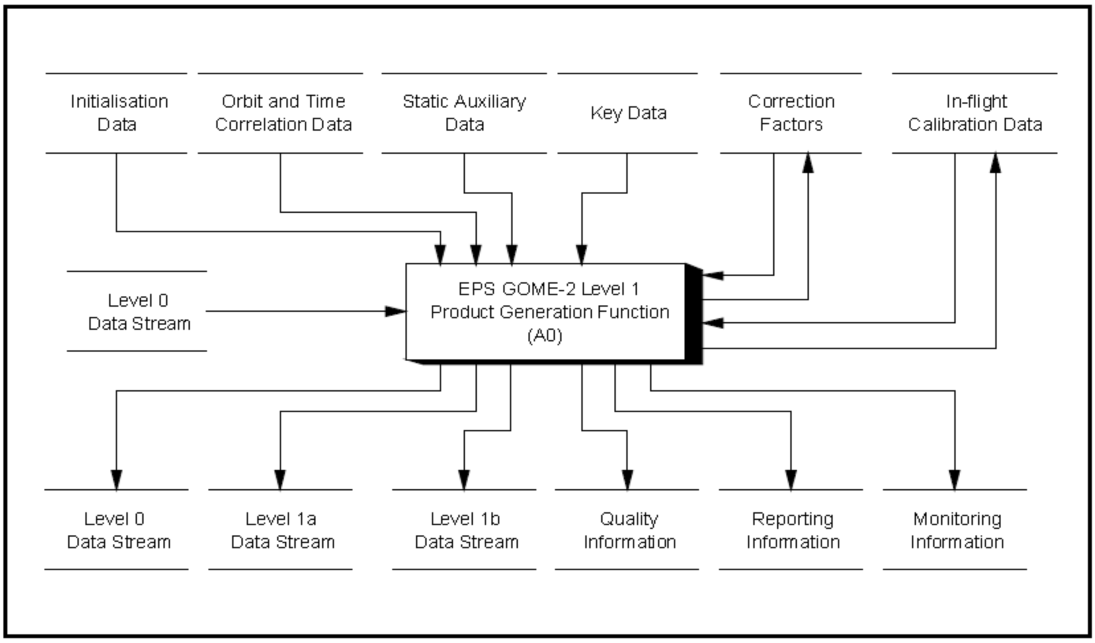

Figure 3: Context Diagram of the GOME-2 Product Generation Function (PGF).

3.1.2.1.1 Inputs

GOME-2 LEVEL 0 DATA STREAM

Level 0 data, the instrument science packets, will be provided to the level 0 to 1a processor as a continuous stream of data packets. In the case of reprocessing this data stream is replaced by the level 0 products which have been generated in a previous run of the level 0 to 1a processor.

INITIALISATION DATA

This data set contains all parameter settings for the PGF, such as threshold values, switches between algorithm options, and instrument parameters not contained in the pre-flight calibration key data.

ORBIT AND TIME CORRELATION DATA

For Near Real Time processing a predicted orbit state vector is required as input for the geolocation calculations. During re-processing restituted orbit data are expected to be available. Time correlation information for the calculation of the UTC time grid are provided as external parameters if required by selection of Determine UTC Time Grid (A2.3.2), Option 3.

STATIC AUXILIARY DATA

The static auxiliary data comprises the static databases that are required for use in the level 0 to 1b processor. They are required in particular for the calculation of geolocation on a fixed grid, the check for sunglint, and effective cloud cover and cloud top pressure determination.

KEY DATA

The Key data comprises the complete set of pre-flight calibration data which is supplied by the instrument provider.

CORRECTION FACTOR DATA

Instrument characteristics such as radiance and irradiance sensitivity will change during the GOME-2 lifetime due to in-orbit degradation of the instrument. Correction factors will be derived in the SPA module (see below) using in-flight measurements and will be made available to the PGF. These data will not be available at the beginning of the in-orbit life of GOME-2. Therefore, the processor must be able to run without them.

IN-FLIGHT CALIBRATION DATA

The level 0 to 1a processing includes the determination of in-flight calibration parameters. From measurements of the various calibration sources encountered during each run of the processor, new calibration constants are calculated and written into an in-flight calibration data storage location. They are also retained in memory for use in processing those data acquired after the satellite comes out of the dark side of the orbit and before the next dump. Calibration parameter *usage* will be updated at the terminator. The terminator is defined by a solar zenith angle in the Northern hemisphere supplied as part of the initialisation dataset. The solar zenith angle will be decreasing as the satellite approaches the terminator. Calibration parameters will be stored for the lifetime of the mission.

3.1.2.2 Outputs

GOME-2 LEVEL 0 DATA STREAM
In case of NRT processing the level 0 to 1a processor gathers the instrument science packets from the level 0 data stream and appends appropriate header information as specified in [AD4] and [AD5]. These data will be stored in the UMARF and are available for reprocessing purposes.

GOME-2 LEVEL 1A DATA STREAM
Depending on the time coverage of the level 0 data stream on input the generated level 1a data stream covers the corresponding time period. The level 0 to 1a processor generates the Level 1a data stream for formatting as specified in [AD4] and [AD5]. These data will be stored in the UMARF and are available for reprocessing purposes.

GOME-2 LEVEL 1B DATA STREAM
Depending on the time coverage of the level 1a data stream on input the generated level 1b data stream covers the corresponding time period. The level 1a to 1b processor generates the Level 1b data stream for formatting as specified in [AD4] and [AD5].

MONITORING INFORMATION
Monitoring information consists of housekeeping data and spectral data, along with their respective time-tags and geolocation. The default sampling interval is one instrument science data packet. Housekeeping data and selected earthshine data are extracted from the level 1 product files. In-flight calibration data are extracted from the in-flight calibration data storage location. Housekeeping data are converted from binary units to physical units. Spectral data are preprocessed according to the instrument mode. All monitoring data are then stored for the lifetime of the mission for later use.

QUALITY INFORMATION
The Product Quality Evaluation (PQE) functionality shall provide information about the quality of the generated level 1 data products. A number of checks are performed during Level 0 to 1a Processing (A2) and Level 1a to 1b Processing (A3) and the results are stored in Product Confidence Data records (PCDs) in the Level 1a and Level 1b data products. PCDs are provided both at the product and scan level. PCDs containing information about the quality of applied calibration parameters is also included. A pre-processing functionality extracts the PCDs directly after processing of the level 1a and 1b data products and updates the PQE storage location with the extracted data. A second functionality further condenses the extracted data to provide daily, weekly, monthly and yearly Product Quality Summaries and “Quick-Look” information. Quality information is stored for the lifetime of the mission. The highest level of detail, on measurement pixel level, is not covered by automatic PQE functionality.

REPORTING INFORMATION
In this document, reporting information is all information sent through the PGE, on the product generation function, with information on, inter alia, the status of the instrument, data processing functions, processing platforms, and links as appropriate. This means that the information contains all events and command acknowledgements raised by the product generation function.

3.1.3 Components of the Product Generation Function (A0)

The GOME-2 Product Generation Function generates the data that is formatted into level 0, 1a, and 1b data streams.

The first level of functional decomposition of the PGF is shown in Fig. 4 and is followed by a short description of the main components of the PGF and their functionality. A detailed specification is given in Section 5.

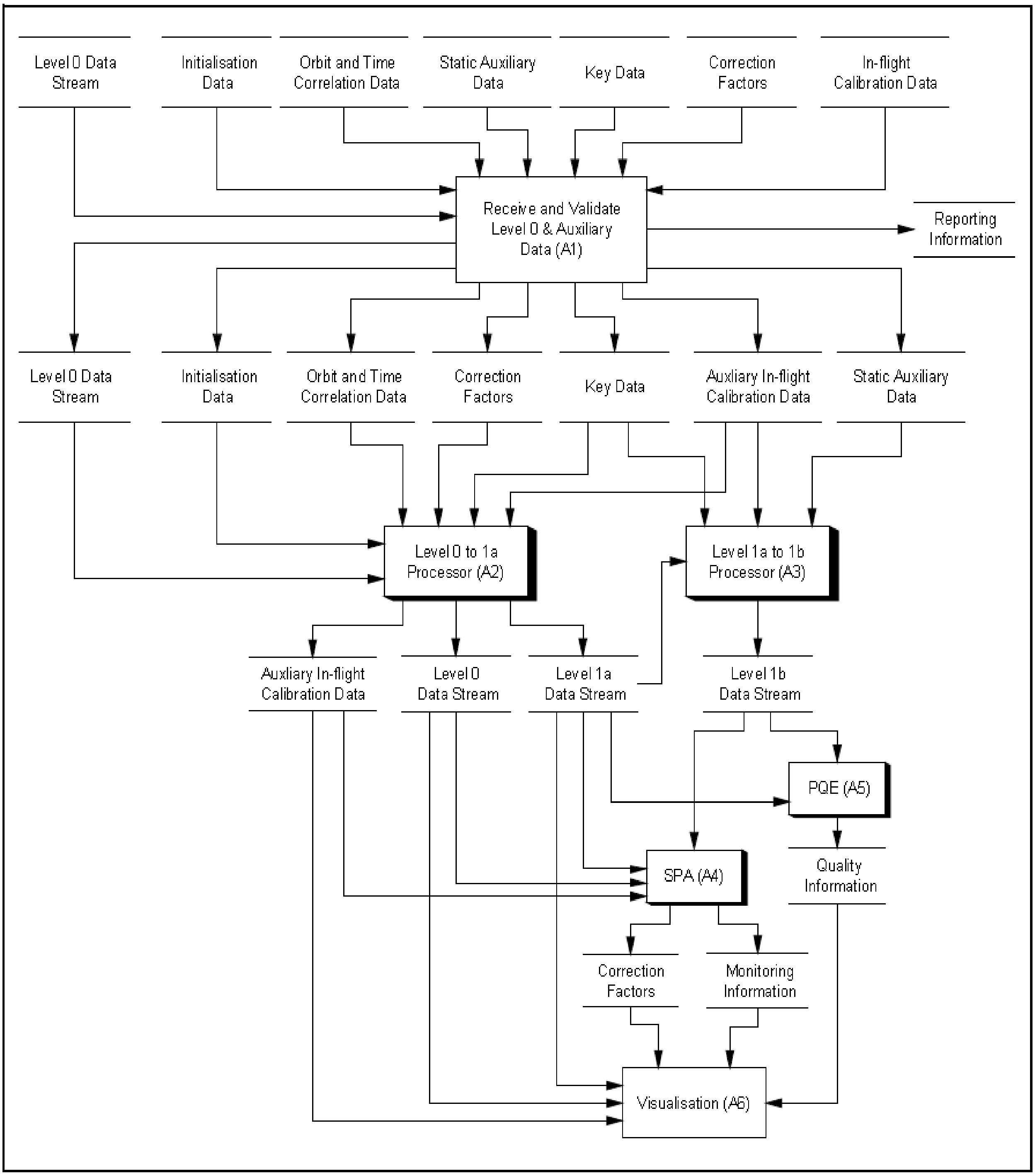

Figure 4: Functional decomposition of the GOME-2 PGF (A0).

RECEIVE AND VALIDATE LEVEL 0 AND AUXILIARY DATA (A1)

The receive and validate functionality, in addition to the generic checks identified in the CGSRD [AD1], performs the instrument-specific acceptance and checking of the input data. Its purpose is to accept the 1evel 0 data and to perform all checks required for validation of the input data before passing them to the algorithmic functions. This functionality correlates level 0 data with auxiliary data and also produces reporting statistics.

LEVEL 0 TO 1A PROCESSING (A2)

The level 0 to 1a processing comprises both the determination of geolocation information on a fixed time grid from the appropriate orbit and attitude information and time correlation information, and the determination of applicable calibration parameters. From measurements of the various calibration sources encountered during each run of the processor, new calibration constants are calculated and written into an in-flight calibration data storage location. They are also retained in memory for use in processing those data acquired after the satellite comes out of the dark side of the orbit and before the next dump. Calibration parameter usage will be updated at the terminator. The terminator is defined by a solar zenith angle in the Northern hemisphere supplied as part of the initialisation dataset. The solar zenith angle will be decreasing as the satellite approaches the terminator. Calibration parameters are expected to be stored in the in-flight calibration data storage location for the lifetime of the mission. Note, any application of calibration parameters in the level 0 to 1a processing should be regarded as interim, to facilitate the generation of new calibration parameters and correction factors. There is no application of calibration parameters to FPA earth observation measurements. The output of the level 0 to 1a processor is to be formatted into the level 0 and 1a products as specified in [AD 4] and [AD 5].

LEVEL 1A TO 1B PROCESSING (A3)

The level 0 to 1b processing comprises the calculation of geolocation parameters for the actual integration time of each measurement, and the conversion of the raw binary readouts on the level 1a data stream to calibrated radiance and irradiance data to be formatted into the level 1b product as specified in [AD 4] and [AD 5].

SENSOR PERFORMANCE ASSESSMENT (SPA) (A4)

The Sensor Performance Assessment (SPA) functionality shall allow instrument performance to be monitored for the lifetime of the mission. Performance shall be monitored both from an engineering point of view, utilising selected housekeeping data, and from a scientific point of view utilising spectral data, in particular in-flight calibration data. The PGF will record monitoring measurements in the level 1a data stream as specified in [AD 4] and [AD 5]. The SPA functionality comprises extraction and preprocessing of the monitoring parameters. The extracted and preprocessed monitoring parameters are stored in the SPA data storage location and made available for further analysis and visualisation. Monitoring parameters for a given time frame are then retrieved from the SPA data storage location and further analysed. Degradation correction factors are calculated where appropriate. The generation of correction factors will be done asynchronously from the product processing and will require an external operator. The SPA data storage location will be maintained for the lifetime of the mission, comprising all MetOp satellites.

PRODUCT QUALITY EVALUATION (A5)
The Product Quality Evaluation (PQE) functionality shall provide information about the quality of the generated level 1 data products. A number of checks are performed during Level 0 to 1a Processing (A2) and Level 1a to 1b Processing (A3) and the results are stored in Product Confidence Data records (PCDs) in the Level 1a and Level 1b data products. PCDs are provided both at the product and scan level. PCDs containing information about the quality of applied calibration parameters are also included. A pre-processing functionality extracts the PCDs directly after processing of the level 1a and 1b data products and updates the PQE storage location with the extracted data. A second functionality further condenses the extracted data to provide daily, weekly, monthly and yearly Product Quality Summaries and "Quick-Look" information. The data generated by the PQE functionality are made available for further analysis and visualisation. The highest level of detail, on measurement pixel level, is not covered by automatic PQE functionality. The PQE data storage location will be maintained for the lifetime of the mission, comprising all MetOp satellites.

VISUALISATION (A6)
The GOME-2 PGF will include a visualisation functionality capable of accepting level 0, level 1a and level 1b data products.

3.2 Operations Concept

3.2.1 Introduction

This section provides an overview of the functionality implemented by the GOME-2 level 0 to 1b processing functionality. Table 2 that follows provides the application domain and behaviour in operational situations.

Operational Situation	*Handling/Behaviour of the Algorithms*	*Impact on Product*
Nominal NRT mode	Fully nominal product extraction	Nominal quality products
Backlog Processing	Fully nominal product extraction. Please see the CGSRD [AD1] for the definition of backlog processing.	Nominal quality products
Reprocessing	Fully nominal product extraction. Please see the CGSRD [AD1] for the definition of peprocessing.	Nominal quality products
Corrupted Level 0 data	In the case of corrupted level 0 data a report is raised to the MCS as specified in Section 5.1. Corrupted data are not further processed.	Non-nominal quality product containing corrupted data flags as specified in Section 5.1 and formatted in [AD4] and [AD5].
Missing Level 0 data	In the case of missing level 0 data a report is raised to the MCS as specified in Section 5.1. Data are processed as specified in Section 5.	Non-nominal quality product containing missing data flags as specified in Section 5 and formatted as specified in [AD 4] and [AD 5].
Missing Initialisation data	In the case of missing initialisation data, halt processing and raise a report to the MCS as specified in Section 5.1.	No product derived. When initialisation data are available process as per backlog processing
Missing Orbit data	In the case of missing orbit data, halt processing and raise a report to the MCS as specified in Section 5.1.	No product derived. When orbit data are available process as per backlog processing.
Missing Time Correlation data	In the case of missing external time correlation data for UTC option 3 in A2.3.2, a report is raised to the MCS as specified in Section 5.1 Data are not further processed.	No product derived. When time correlation data are available process as per backlog processing.
Missing Static Auxiliary data	In the case of missing auxiliary data, raise a report to the MCS as specified in Section 5.1 and continue processing specified in Section 5.	Non-nominal quality product containing a missing static auxiliary data flag as specified in Section 5.1 and formatted in [AD 4] and [AD 5]. No cloud parameters are derived. When static auxiliary data are available process as per reprocessing.
Missing Pre-Flight Calibration Key data	In the case of missing pre-flight calibration key data, halt processing and raise a report to the MCS as specified in Section 5.1.	No product derived. When preflight calibration key data are available process as per backlog processing.
Missing Correction Factor data	In the case of missing correction factor data, raise a report to the MCS as specified in Section 5.1 and continue processing specified in Section 5.	Nominal quality product containing a missing correction factor data flag as specified in Section 5.1 and formatted in [AD 4] and [AD 5].

Operational Situation	*Handling/Behaviour of the Algorithms*	*Impact on Product*
Missing In-flight Calibration Key data	In the case of missing in-flight calibration key data, halt processing and raise a report to the MCS as specified in Section 5.1.	No product derived. When inflight calibration key data are available process as per backlog processing.
Invalid Date for In-flight Calibration data	In the case of in-flight calibration data whose validity date has expired, raise a report to the MCS as specified in Section 5.1 and continue processing as specified in Section 5.1.	Non-nominal quality product containing an invalid date auxiliary data flag as specified in Section 5.1 and formatted in [AD 4] and [AD 5]. When valid data are available process as per reprocessing.
Duplicate data	Duplicate data are discarded, latest data are kept.	Nominal quality products
Wrong satellite or instrument	In the case of wrong satellite or instrument data, halt processing and raise a report to the MCS as specified in Section 5.1.	No product derived.

Table 2: Domain of Application and Behaviour in Operational Situations.

3.2.2 Near-Real Time Mode

It is foreseen that the GOME-2 will be operated continuously. GOME-2 has a variety of observation modes as outlined in Section 2.3.3. The operational PGF level 0 to 1a and level 1a to 1b processing functionality must run for 24 hours per day, fully automatically for the full mission life of the EPS programme. In doing so, it must process all the science data packets from GOME-2, all ancillary data from the instrument and platform as appropriate, and all necessary auxiliary data, received via the PGE, for all the instrument's operational modes.

3.2.3 Backlog Processing

Please see the CGSRD [AD 1] for the definition of Backlog Processing.

3.2.4 Reprocessing

Please see the CGSRD [AD 1] for the definition of Reprocessing.

4 REQUIREMENTS LISTING

4.1 Detailed System Components

The following notes on detailed system components are to be understood in the context of Section 5. They are presented here for convenience only. For detailed descriptions, please refer to Section 5. The component numbers listed below are references to the functional components presented therein and are used in subsequent identification of requirements following the convention:

ALG-TYP-NNN-AX.XX.X

where **ALG** stands for algorithm requirement, **TYP** refers to the type of requirement as specified in the appropriate section headings, **NNN** is the number of the requirement and **Ax.xx.x** is the number of the component as listed below.

Notwithstanding the use of terms including "function" and "sub-function" below, nothing in this section shall be taken as constraining the details of the implementation, as opposed to the functionality of the PGF.

Table 3 that follows lists the system components as used for definitions of system requirements.

Number	*Configuration Item*
A1	**Receive and Validate Level 0 and Auxiliary Data** In addition to the generic checks identified in the CGSRD [AD1] the functionality that performs the instrument-specific acceptance and checking of the input data is required. Its purpose is to accept the level 0 data, check their integrity, and to perform all checks required for validation of the input data before passing them to the algorithmic functions.
A1.1	**Receive & Validate Level 0 Data Flow** This functionality encompasses the check and validation of the level 0 data flow from the instrument. The generic checks identified in [AD1] are followed by the verification against the expected instrument/ SC configuration. The GOME-2 level 0 data flow is checked in three steps, of which the first two are related to the integrity of individual packets, and the last one to the integrity of the sequence of packets. • GOME-2 data packets are identified in the data flow via their fixed fields. The length of the data packets is checked. • For each packet, the checksum is recalculated and compared against the checksum contained in the packet. • A basic check for duplicate packets and the time order of the packets is performed.
A1.2	**Receive, Validate and Correlate Side Information** This functionality receives the side-information, validates them and relates them to the level 0 dataflow. It shall be checked that all input data which are needed besides the level 0 data flow (see Section 5.2.1 for a list) are available. Should any of them be missing, a report shall be raised via the MCS, and the processing cannot continue. In the case that some of the in-flight calibration data selected are older than a specified threshold, a report shall be raised via the MCS, the processing shall continue using these data, and the products shall be flagged as degraded. The checks on the individual input data are not performed here, but after they have been read (A2.0).
A2	**Level 0 to 1a Processing** The level 0 to 1a processor will accept a level 0 data stream and the corresponding auxiliary data comprising initialisation data, orbit data, key data, correction factor data, and in-flight calibration data and generates one level 1a and one level 0 output data stream. The level 1a and 0 data stream on output will have the same coverage.
A2.0	**Read Input Data** All input data will be read by the level 0 to 1 processor in accordance with the following sub-components.
A2.0.1	**Read Initialisation Data** The Initialisation Data listed in Section 5.2.2.3 are read from the Initialisation Data storage location and made available for use in ‘Level 0 to 1a Processing (A2)’.

Number	*Configuration Item*
A2.0.2	**Read Orbit and Time Correlation Data** The Orbit and, if required by selection of ‘Determine UTC Time Grid (A2.3.2): UTC option 3’, Time Correlation Data listed in Section 5.2.2.3 are read from the Orbit and Time Correlation Data storage location and made available for use in ‘Calculate Geolocation for Fixed Grid (A2.6)’ and ‘Determine UTC Time Grid (A2.3.2)’.
A2.0.3	**Read Static Auxiliary Data** The Static Auxiliary Data listed in Section 5.2.2.3 are read from the Static Auxiliary Data storage location and made available for use in ‘Level 0 to 1a Processing (A2)’.
A2.0.4	**Read Key Data** The Key Data listed in Section 5.2.2.3 are read from the Key Data storage location and made available for use in ‘Preprocess Müller Matrix Elements (A2.1)’.
A2.0.5	**Read Correction Factor Data** The Correction Factor Data listed in Section 5.2.2.3 are read from the Correction Factor Data storage location and made available for use in ‘Preprocess Müller Matrix Elements (A2.1)’.
A2.0.6	**Read In-flight Calibration Data** The In-flight Calibration Data listed in Section 5.2.2.3 are read from the In-flight Calibration Data storage location and made available for use in ‘Level 0 to 1a Processing (A2)’.
A2.0.7	**Read Level 0 Input Data, Separate Scans and Generate PCDs** The level 0 data stream associated with one product is read and made available for use in ‘Level 0 to 1a Processing (A2)’. The data stream is split into individual scans each comprising a maximum of 16 data packets. The first data packet in a complete scan is indicated by a data packet subset counter of zero, $sub = 0$. The last data packet in a scan is indicated by a data packet subset counter of 15, $sub = 15$. The data packet subset counters of intervening data packets are incremented by 1 per data packet.
A2.1	**Preprocess Müller Matrix Elements** This functionality calculates the Müller Matrix elements (see Appendix E and E.2) from the Calibration Key Data. The calculation of MMEs is done once only as a pre-processing step before the processing of measurement data starts. The MMEs are corrected with M-factors which account for the in-flight degradation of instrument behaviour. When new correction factor data become available the new M-factors must be applied to the precalculated MMEs but the MMEs themselves need not be recalculated. The update in usage of the newly corrected MMEs occurs at the start of processing a complete product. They are subsequently interpolated to a fine grid of viewing angles, and solar azimuth and elevation angles. Those interpolated MMEs which are also needed for Level 1a to 1b processing are output to the Level 1a product, with their errors.

Number	*Configuration Item*
A2.2	**Convert Housekeeping Data** See corresponding component AG.4
A2.3	**Determine Observation Mode and Viewing Angles.** Derive the observation mode and the viewing angles for a scan from a combination of housekeeping data. Data from different observation modes will be sent to different branches of the 0 to 1b processing. This modules derives the observation mode for a scan from a combination of housekeeping data and viewing angles. The viewing angles themselves are calculated from the scan mirror readings in the data packet. Scans which do not match any of the available observation modes are classified as "invalid". Furthermore both the PMD transfer and readout mode are determined, and the UTC times corresponding to the scan mirror positions are calculated.
A2.4	**Determine PCDs from Raw Intensity** This functionality applies generic saturation and hot pixel checks to the raw intensity. Saturation checks are applied to data from all measurement modes with the exception of PMD data transferred in *band + raw* or *band + mixed* mode. Hot pixel checks are applied only to data from *dark*, *LED* and *WLS* observation modes.
A2.5	**Prepare PMD Data** See corresponding component AG.5
A2.6	**Calculate Geolocation for Fixed Grid** The objective of the Geolocation function is to calculate a set of geolocation parameters (depending on the instrument mode) from an orbit state vector, the UTC, and scanner viewing angles. A common basic set of geolocation parameters is calculated for all measurement modes. This includes the latitude and longitude of the sub-satellite point (SSP), and the solar zenith and azimuth angles at the satellite. For the earth observation, sun and moon modes, additional parameters specific to these modes are calculated: • For earth observation measurements, solar and line-of-sight zenith and azimuth angles at a given top-of-atmosphere height, the corner and centre coordinates of the ground pixel at ground level, the satellite height, and the earth radius are calculated. • For solar measurements, the distance between satellite and sun and the velocity component towards the sun are calculated. • For lunar measurements, a number of parameters describing the lunar measurement geometry are calculated. All geolocation calculations expect on input an orbit state vector (mean Kepler elements at true ascending node crossing) and the time for which the calculation shall be performed. In addition, the calculations for earthshine measurements need the scanner viewing angles and the size of the IFOV.

Number	*Configuration Item*
AG.2.1	**Determine Sub-Satellite Point** In this module, latitude, longitude, and satellite height are calculated on a 187.5 ms grid synchronised with every second scanner position, for k = 0, 2,…, 60, 62 (32 times per scan). Distances to sun and moon and sunlit area of the moon vary only little during a scan, so only one value (at k = 0) is returned. The orbit propagator must have been successfully initialised (AG.1) such that the epoch of the ascending node crossing t_{ANX} and the requested time for prediction t_P are within two nodal periods. These are calculations of satellite parameters, not GOME-2 scanner viewing angles.
AG.2.2	**Calculate Line-of-Sight Angles for the Ground Footprint** These calculations are performed for the Earth observation mode only. Their purpose is to derive from the scanner viewing angle and the IFOV dimensions the LOS elevation and azimuth angles in the Satellite Relative Actual Reference CS. These angles are needed in the next step (Calculate Target Pointing Information) as input to the PGE services. They are not reported in the product.
AG.2.3	**Calculate Target Pointing Information** The calculations to be performed here depend on the instrument mode. • Earth observation modes: Calculations are performed for all ground pixels (n = 0…31) and points within a ground pixel (m = A…G) see Figure 18. If m = A, B, C, D the ground pixel corner latitude/longitude coordinates are calculated. If m = F the ground pixel centre latitude/longitude coordinates are calculated. If m = E, F, G the satellite and solar elevation and azimuth angles are calculated. • Solar mode: Solar azimuth and elevation in the Satellite Relative Actual Reference CS are calculated here. • Lunar mode: Lunar azimuth and elevation in the Satellite Relative Actual Reference CS are calculated here. Lunar parameters are calculated for the start of the scan only (k = 0). The distances between moon and sun and between moon and satellite are also determined here.
A2.7	**Determine PCDs from Geolocation** This functionality applies generic SAA, sunglint and rainbow checks to data from all measurement modes on the basis of geolocation and viewing information calculated in Calculate Geolocation for Fixed Grid (A2.6). These checks are applied to all data including those that may later be excluded from the processing on the basis of subsequent quality checking.
A2.8	**Calculate Dark Signal Correction** To calculate dark signal correction parameters on the basis of all measurements made in *dark* calibration mode, on the dark side of the orbit. The calculation of the dark signal correction requires all scans taken during the *dark* calibration mode to be collected. As the measured dark signal is dependent on both integration time and detector temperature, the accumulated scans must be sorted on the basis of integration time and into detector temperature bins. Data must also be sorted into all combinations of PMD readout and transfer mode as specified in Appendix B. The dark signal correction is calculated as the mean of all *dark* detector pixel readouts for each channel/band. The readout noise is calculated as the standard deviation of the *dark* detector pixel readouts for each channel/band.

Number	*Configuration Item*
A2.9	**Apply Dark Signal Correction** See corresponding component AG.11
A2.10	**Normalise Signals to One-Second Integration Time** See corresponding component AG.12
A2.11	**Calculate PPG** To determine the Pixel to Pixel Gain (PPG) correction using measurements taken in *LED* calibration mode. Adjacent pixels on an array detector may have slightly different Quantum Efficiency otherwise known as Pixel to Pixel Gain (PPG). This PPG pattern is superimposed on all other calibration and earthshine measurements. It is necessary to remove the PPG gain before proceeding further with the processing of calibration measurements. PPG is determined using measurements taken in *LED* calibration mode anticipated to be part of the monthly calibration timeline. When GOME-2 is in *LED* calibration mode the detector arrays are illuminated with light from on-board LEDs without spectral dispersion. Deviations from spectrally smooth behaviour in the measurements may be attributed to PPG.
A2.12	**Apply PPG Correction** See corresponding component AG.13
A2.13	**Calculate Spectral Calibration Parameters for Main Channels** GOME-2 spectra are acquired by linear diode array detectors. The spectrum is dispersed across the diode array, so that each detector pixel (centre) corresponds to a particular wavelength. Spectral calibration is the assignment of a wavelength value to each detector pixel. For each GOME-2 channel, a low order polynomial approximation will be used to describe wavelength as a function of detector pixel. This module derives the polynomial coefficients for the main channels from preprocessed spectra of the Spectral Light Source (SLS) which provides a number of narrow spectral lines at known wavelengths across the GOME-2 wavelength range.
A2.14	**Calculate Spectral Calibration Parameters for PMD Channels** This module derives the polynomial coefficients describing the spectral dispersion of the PMD channels from preprocessed spectra of the Spectral Light Source (SLS). The module (AG.14) will later on calculate the wavelength for each detector pixel from these polynomial coefficients. See Section 5.2.15 for a general introduction to wavelength calibration of GOME-2 spectra. The algorithm used for the PMD channels is different from the one used for the main FPA channels, because at the lower spectral resolution of the PMD channels individual spectral lines of the SLS cannot be resolved. Instead, an expected PMD spectrum is calculated from the main FPA signals. The spectral shift between expected and measured PMD spectrum is then determined by cross-correlating the two in a number of predefined spectral windows.
A2.15	**Apply Spectral Calibration Parameters** See corresponding component AG.14.

Number	*Configuration Item*
A2.16	**Calculate Etalon Correction** This module calculates an Etalon correction using measurements taken in the *WLS* calibration mode. Etalon is an interference phenomenon, which arises in the thin protective layer coated on the detector chip. This causes a wave-like pattern on the radiance response, where the position of the minima and maxima of the wave depend on the ratio between layer thickness and wavelength. The polarisation sensitivity of the instrument is not affected. At the shortest wavelengths in channel 1 we expect (based on ERS-2/GOME experience) approximately 10 minima and maxima over the channel (i.e. the interference wave has a wavelength of around 100 pixels). At the longest wavelengths of the channel 4 this number reduces proportionally with wavelength to around 4 (i.e. 250 pixels per interference wavelength).
A2.17	**Apply Etalon Correction** See corresponding component AG.15
A2.18	**Determine Straylight Correction** See corresponding component AG.16
A2.19	**Apply Straylight Correction** See corresponding component AG.17
A2.20	**Calculate SMR** This module calculates a Solar Mean Reference spectrum (SMR) on the basis of detector readouts measured during Sun calibration mode. During the Sun calibration mode, the Sun moves through the FOV of the diffuser in elevation direction. The solar calibration timeline will start before the Sun is fully in the field-of-view of the diffuser, and end after the Sun has left the FOV. Only those detector readouts for which the Sun is fully in the FOV are used in the calculation of the SMR. Selection is based on solar elevation angle. Only those measurements within a pre-specified range of the central elevation angle are selected. To check that the correct sequence have been selected, a pair-wise intensity check is made on measurements on either side of the middle of the selected sequence. If the deviation from the central spectrum is too large both readouts are discarded. Furthermore, those readouts which do not correspond to a complete band 1a readout are also discarded. The Solar Mean Reference spectrum (SMR) is calculated as the average, after application of the irradiance response of the instrument, of all selected detector readouts which have passed the intensity check during the solar calibration period. In addition the precision error on the SMR is calculated.
A2.21	**Determine Stokes Fractions** Calculate Stokes fractions from measurement geometry and preprocessed PMD measurements. GOME-2 is a polarisation-sensitive instrument. The measured signals are determined by the total intensity and the polarisation state of the incoming light. The 0 to 1b processor has the task to derive the total intensity from the measured signals. Therefore the polarisation state of the incoming light has to be characterised. This will be done by this module, utilising the measurements of the PMD channels.

Number	*Configuration Item*
A2.22	**Collect Global PCDs per Product** All global PCDs are collected at the completion of processing of one complete product, assumed in this context to be 'dump to dump'. Global PCDs are typically flags indicating non-nominal behaviour and cumulative counts of the number of occurrences of non-nominal behaviour. Information describing observation mode statistics is also included. Global PCDs will be written in the level 1a and subsequently the level 1b product.
A2.23	**Write Level 0 and 1a Product** All information to be included in the level 1a product, and additional header information to be included in the level 0, is collated and formatted as specified in [AD 4] and [AD 5].
A3	**Level 1a to 1b Processing** The level 1a to 1b processor will accept a level 1a data stream and the corresponding auxiliary data comprising initialisation data, static auxiliary data and key data and generates one level 1b. The level 1b data stream on output will have the same coverage as the input level 1a data stream.
A3.0	**Read Input Data** All input data will be read by the level 1a to 1b processor in accordance with the following sub-components.
A3.0.1	**Read Initialisation Data (A3.0.1)** The Initialisation Data listed in Section 5.3.2.3 are read from the Initialisation Data storage location and made available for use in 'Level 1a to 1b Processing (A3)'.
A3.0.2	**Read Static Auxiliary Data (A3.0.2)** The Static Auxiliary Data listed in Section 5.3.2.3 are read from the Static Auxiliary Data storage location and made available for use in 'Level 1a to 1b Processing (A3)'.
A3.0.3	**Read Key Data (A3.0.3)** The Key Data listed in Section 5.3.2.3 are read from the Key Data storage location and made available for use in 'Level 1a to 1b Processing (A3)'.
A3.0.4	**Read Level 1a Input Data (A3.0.4)** The level 0 data stream associated with one product is read and made available for use in Level 0 to 1a Processing (A2).
A3.1	**Prepare PMD Data** See corresponding component AG.5
A3.2	**Calculate Geolocation for Actual Integration Times** This module calculates the geolocation information for the ground pixels corresponding to the actual main channel integration times from the geolocation information for the fixed 187.5 ms grid contained in the level 1a product.

Number	*Configuration Item*
A3.3	**Apply Dark Signal Correction** See corresponding component AG.11
A3.4	**Normalise Signals to One Second Integration Time** See corresponding component AG.12
A3.5	**Apply PPG Correction** See corresponding Component AG.13
A3.6	**Apply Spectral Calibration Parameters** See corresponding component AG.14
A3.7	**Apply Etalon Correction** See corresponding component AG.15
A3.8	**Determine Straylight Correction** See corresponding component AG.16
A3.9	**Apply Straylight Correction** See corresponding component AG.17
A3.10	**Apply Polarisation Correction** This module corrects signals measured in the main channels in earth observation mode for the polarisation sensitivity of the instrument. This corresponds to converting the signals to signals which would have been observed with an instrument which is not sensitive to the polarisation state of the incoming radiance, or, equivalently, to signals which would have been observed with unpolarised light on input. Applying polarisation correction is a necessary prerequisite for an absolute radiometric calibration of the earth radiances, i.e., for applying the radiance response function. The module uses the Stokes fractions *q* derived from collocated PMD measurements characterising the polarisation state of the incoming radiance, and the Müller matrix elements m2 for the main channels, characterising the polarisation sensitivity of the instrument.
A3.11	**Apply Radiance Response** To correct *Earthshine* measurements for the radiance response of the instrument. The application of the radiance response is a division of the detector readouts to be corrected by the MMEs describing the radiance response of the instrument. It is assumed that the signals have been corrected for dark current, PPG, Etalon and straylight, and spectrally calibrated. The MMEs describing the radiance response of the instrument are calculated on a fixed wavelength grid at the time of the pre-processing of the MMEs. Furthermore they are pre-calculated for a fine grid of scan angles. The MMEs must first be interpolated to the wavelength grid of the measurement to be corrected and to the appropriate scan angle.

Number	*Configuration Item*
A3.12	**Apply Irradiance Response** See corresponding component AG.18
A3.13	**Correct Doppler Shift** See corresponding component AG.19
A3.14	**Reduce Spatial Aliasing** To correct for the effect of the finite detector pixel readout time which causes individual detector pixels to view slightly shifted ground scenes, an effect referred to as 'Spatial Aliasing' as spatial variability is aliased into spectral variability in the measurements. The detector pixels are read out consecutively and therefore each pixel observes a ground scene that is slightly shifted in space. When the ground scene is changing e.g. in the case of cloud/land/water or water/land transitions, the different detector pixels will observe different ground scenes with different spectral signatures. The principle of the method lies in scaling the main channel detector readouts by the ratio of PMD readouts as they occur during the integration time of the main channels. Since the PMDs have a temporal resolution up to eight times higher than that of the main channels, a representative correction can be obtained by co-adding the PMDs over the integration time of main channel signals and interpolating in time to the exact integration time of each main channel detector pixel.
A3.15	**Calculate Fractional Cloud Cover and Cloud Top Pressure** An effective cloud cover and cloud top pressure is retrieved for each GOME-2 ground pixel using the Fast Retrieval Scheme for Clouds from the Oxygen A band (FRESCO), developed by KNMI ([RD 21] and [RD 21]). The continuum absorption in the region of the Oxygen-A band is principally determined by the cloud fraction, the cloud optical thickness (or cloud albedo) and the surface albedo. In the Oxygen-A band itself the reflectivity depends, in addition, on the cloud top pressure since clouds screen most of the oxygen inside and below them. The absorption within the Oxygen-A band is therefore higher for a ground pixel with low cloud than one with high cloud. Combined information on cloud fraction and cloud optical thickness may be derived from the reflectivity in the continuum and cloud top pressure may be estimated from the depth of the Oxygen-A band.
A3.16	**Collect Global PCDs per Product** All global PCDs, indicated in the variable tables by the type 'g' are collected at the completion of processing of one complete product, assumed in this context to be 'dump to dump'. Global PCDs are typically flags indicating non-nominal behaviour and cumulative counts of the number of occurrences of non-nominal behaviour. Information describing observation mode statistics is also included. All global PCDs included in the level 1a product are also included in the level 1b product.
A3.17	**Write Level 1b Product** All information to be included in the level 1b product is collated and formatted as specified in [AD 4] and [AD 5].

Number	*Configuration Item*
A4	**Sensor Performance Assessment (SPA)** The Sensor Performance Assessment (SPA) functionality shall allow instrument performance to be monitored for the lifetime of the mission. Performance shall be monitored both from an engineering point of view, utilising selected housekeeping data, and from a scientific point of view utilising spectral data, in particular in-flight calibration data. The SPA functionality comprises extraction, preprocessing and analysis of the monitoring parameters. From the analysis, degradation correction factors (m-factors) shall be derived. The monitoring parameters shall be stored in an SPA data storage location.
A4.1	**SPA Extraction and Pre-processing** Monitoring data are extracted from level 1a products, level 1b products, and in-flight calibration files. They are preprocessed and written to the SPA data storage location.
A4.2	**SPA Analysis** Monitoring data for a given time frame are retrieved from the SPA data storage location and further analysed. Degradation correction factors are calculated where appropriate.
A5	**Product Quality Evaluation** The Product Quality Evaluation (PQE) functionality shall provide information about the quality of the generated level 1 data products. A number of checks are performed during Level 0 to 1a Processing (A2) and Level 1a to 1b Processing (A3) and the results are stored in Product Confidence Data records (PCDs) in the Level 1a and Level 1b data products. PCDs are provided both at the product and scan level. PCDs containing information about the quality of applied calibration parameters are also included. A pre-processing functionality extracts the PCDs directly after processing of the level 1a and 1b data products and updates the PQE storage location with the extracted data. A second functionality further condenses the extracted data to provide daily, weekly, monthly and yearly Product Quality Summaries and “Quick-Look” information. The highest level of detail, on measurement pixel level, is not covered by automatic PQE functionality.
A5.1	**PQE Extraction** Header information, all PCD records, and a selected sub-set of Earthshine measurements are extracted from the level 1a and 1b data products as specified in equation [AD4] and equation [AD5], to be used in the generation of Product Quality Summary and “Quick-Look” information. The extracted data are written to the PQE storage location. Initialisation parameters are also read from an initialisation file.
A5.2	**Process Product Quality Information** The data extracted in PQE Extraction (A5.1) is further condensed to provide daily, weekly, monthly and yearly Product Quality Summaries. Daily “Quick-Look” products are also generated. The highest level of detail, on measurement pixel level, is not covered by automatic PQE functionality.

Number	*Configuration Item*
A6	**Visualisation** The Visualisation functionality shall provide all the imaging facilities required for the visualisation of the GOME-2 science data packets, level 0, 1a and 1b products including in-flight calibration data and correction factors. It shall also support the visualisation of the quality information produced by the PQE functionality, and monitoring information produced by the SPA functionality.
AG.1	**Initialise Orbit Propagator** The objective of this module is to ensure that the PGE orbit propagator is correctly initialised for the current orbit state vector.
AG.3	**Calculate MMEs for PMD Data in Band Transfer Mode** In the case of PMD data transferred in *band + mixed* or *band + raw* transfer modes MMEs and their errors which are band averaged should be used. In this case it is necessary to calculate the MMEs and their ratios as the mean value over the PMD bandwidth. Mean errors are also calculated as appropriate. This is done by integrating the MMEs in question over the wavelength range associated with each PMD band. These calculations need only be repeated if the PMD band definition is changed.
AG.4	**Convert Housekeeping Data** This module converts selected GOME-2 housekeeping data from the raw instrument binary units into engineering units. Only those data which are relevant to the 0 to 1b processing are converted. These are (as a minimum) predisperser prism and detector temperatures, and lamp currents and voltages. For the conversion, polynomial coefficients from the GOME-2 TM/TC data sheets [AD 6] have to be used.
AG.5	**Prepare PMD Data** If GOME-2 uses PMD band transfer (see Appendix B), PMD readouts are spectrally co-added into 15 bands and divided by co-adding factors before they are transmitted to ground. The co-adding factors are selected such that the result fits into a 2-byte word. They are reported (as exponents to the base of 2) in the PMD status words of the Science Data Packet. This module reconstructs the PMD band signals by multiplying the signals in the Science Data Packet with their respective co-adding factors. This is the first processing step to be applied on PMD band data.
AG.6	**Check for Saturated Pixels** The objective of this module is to check for detector pixel saturation on the basis of pre-specified threshold values supplied per channel/band as input. If a detector pixel read-out exceeds a certain limit specified in the initialisation file for each channel/band it is regarded as being saturated. A saturation mask is generated per channel/band for each readout in the scan. Channel/bands affected by saturation are excluded from further processing. Further, a flag is set per scan and channel/band if saturated pixels are detected in any readout in the scan.

Number	*Configuration Item*
AG.7	**Check for Hot Pixels** Generation of a hot pixel mask is done on the basis of pixel in tensity. A hot pixel threshold is pre-specified as one value per channel/band. A pixel is discarded from the calibration processing if its value deviates from that of the neighbouring pixels by more than the threshold value. The neighbouring pixels at either side of the hot pixel are also discarded. A flag is set per channel/band if hot pixels are detected in any of the readouts in the scan.
AG.8	**Check for SAA** To determine whether measured data lies in the SAA anomaly. The SAA region will be specified as a rectangular region in longitude and latitude. Calibration mode data measured in the SAA will not be used in calibration processing.
AG.9	**Check for Sunglint** Sunglint is a phenomenon that invalidates the calculation of air mass factors in level 2 processing and must be flagged during Level 0 to 1a Processing (A2). Two thresholds for medium and high sunglint danger will be used. Sunglint is strongly dependent on the observing geometry. The flag simply indicates a geometrical possibility. The check is evaluated for shortest effective integration time of the main channels (187.5 ms, 32 times per scan) independent of the actual integration time. Line of sight angles have been calculated previously in Calculate Geolocation for Fixed Grid (A2.6).
AG.10	**Check for Rainbow** Rainbow is a phenomenon which may result in high polarisation above water clouds. As this may invalidate assumptions made in the interpolation of fractional polarisation parameters it must be flagged during Level 0 to 1a Processing (A2). Rainbow is strongly dependent on the observing geometry. The flag simply indicates a geometrical possibility. The actual presence of reflecting surface (water or clouds) is not checked. The check is evaluated for shortest effective integration time of the main channels (187.5 ms, 32 times per scan) independent of the actual integration time. Line of sight angles have been calculated previously in Calculate Geolocation for Fixed Grid (A2.6).
AG.11	**Apply Dark Signal Correction** The dark signal correction is dependent on integration time, detector temperature, PMD transfer and PMD readout mode, therefore the dark signal correction appropriate to the measurement integration time, detector temperature, PMD transfer and PMD readout mode must be selected from the auxiliary calibration data. All individual readouts in the input scan data are separated and then corrected for dark signal by subtraction of the selected dark signal correction.
AG.12	**Normalise Signals to One-Second Integration Time** This module normalises all signals previously corrected for Dark Signal to an effective Integration Time of one second. The signal detector readouts and their errors must at a minimum have been previously corrected for dark signal. Other calibration corrections may or may not have been applied as required. The detector signal readouts and their errors are normalised to an effective integration time of one second through division by the Integration Time specified in seconds.

Number	*Configuration Item*
AG.13	**Apply PPG Correction** This module corrects all measurements, excluding those from *dark* and *LED* calibration modes for PPG. The PPG correction is applied only after the correction for dark signal and normalisation to one second integration time. All individual readouts in the input scan are separated. The PPG correction for each detector pixel of each channel/band is applied by dividing each detector pixel readout by the corresponding pixel of the PPG correction. The error on PPG adds to the noise which has been calculated in the application of dark signal. It is based on an estimate of the error in the pixel to pixel gain correction provided as part of the initialisation data.
AG.14	**Apply Spectral Calibration** This module assigns a wavelength to each detector pixel of the main channels and the PMD channels. This is in fact the only calibration step which is not applied to the measured signals. The module uses the pre-calculated spectral calibration parameters from modules Calculate Spectral Calibration Parameters for Main Channels (A2.13) and Calculate Spectral Calibration Parameters for PMD Channels (A2.14) which are the polynomial coefficients for the conversion from detector pixel numbers to wavelengths.
AG.15	**Apply Etalon Correction** The Etalon correction is applied only after the correction for dark signal, normalisation to one second integration time and PPG correction. All individual readouts are read from the scan. The Etalon correction must be interpolated from its own wavelength grid to that of the measurement to be corrected. This is done using Spline Interpolation (AX.3). The Etalon correction for each detector pixel of each channel/band is then applied by dividing each detector pixel readout by the corresponding pixel of the interpolated Etalon correction.
AG.16	**Determine Straylight Correction** To generate a straylight correction on the basis of measured detector readout intensity and straylight characterisation parameters determined on-ground. Straylight refers to the component of measured intensity for any given detector pixel, which originates from a wavelength other than that associated with that detector pixel. Two types of straylight will be considered, uniform straylight and ghost straylight. Uniform straylight originates in diffuse scatter inside the instrument and generates a slowly varying or nearly uniform straylight across a detector array. Ghost straylight originates in specular reflections from optical components within the instrument. It is essentially focused on the detector array. One channel may contain several ghosts. Each ghost in a channel is associated with a parent detector pixel location. The wavelength assigned to the parent detector pixel is the wavelength associated with the ghost intensity. The ghost straylight correction for each detector pixel is a summation of scaled intensities from all contributing parent locations in the channel. Each ghost location is specified in the calibration Key Data as a polynomial function of parent pixel for each channel/band The intensity of each ghost is specified as a polynomial function of parent pixel, subsequently scaled by the parent pixel intensity.
AG.17	**Apply Straylight Correction** All measurements taken in *Sun observation* mode and *Earth* mode are corrected for straylight. The measured signal is corrected for straylight by subtraction of the straylight correction. It is assumed that the measured signal has previously been corrected for dark signal, normalised to one second integration time, corrected for PPG, Etalon and in addition has been spectrally calibrated.

Number	*Configuration Item*
AG.18	**Apply Irradiance Response** The aim of this module is to correct *Sun* observation mode measurements for the irradiance response of the instrument and to calculate both the total absolute error and the contribution due to random noise.
AG.19	**Correct Doppler Shift** This module corrects the Doppler shift on measured solar spectra using the relative speed of satellite and sun. The solar spectrum with the corrected wavelength axis is the one GOME-2 would have observed if the satellite had not moved relative to the sun. Doppler correction of the solar spectra aligns the spectral features (in particular, the Fraunhofer lines) of solar and earthshine spectra which is an important prerequisite for ratioing them.
AG.20	**Calculate Centre Coordinates** This module calculates geodetic latitude and geocentric longitude of the point at the centre of the geodesic line between two points specified by their geodetic latitude and geocentric longitude.
AX.1	**Calculate Mean, Standard Deviation and Mean Error of Readouts** To generate a mean readout value, standard deviation, and error on the mean from a number of input detector array readouts and their associated absolute error and noise values. A combined saturation and hot pixel mask is applied to each detector readout before calculation begins.
AX.2	**Linear Interpolation** This module describes linear interpolation which calculates the interpolated values by applying a simple straight line connecting adjacent data points. The following algorithm applies to both evenly and unevenly separated data points.
AX.3	**Spline Interpolation** The objective of Spline interpolation is to fit a smooth curve through a set of points based on local polynomial in such a way that the 1st derivative is smooth and the 2nd order derivative is continuous.
AX.4	**Akima Interpolation** The Akima method attempts to produce a curve through a set of data points so the resultant curve will appear smooth and natural, like one drawn manually. The method does not assume any functional form for the curve, but the slope of the curve is determined locally and the interpolation between two successive points is represented by polynomial of degree three, at most. The polynomial is determined from the coordinates of and the slopes at the two points. Since the curve slope must also be determined at the end points of the curve, estimation of two more points is necessary at each end point.

Table 3: System components used for definition of system requirements.

4.2 High Level Requirements

ALG-HGH-005-A0

The product generation function shall support all modes of operation identified in the CGSRD [AD 1] and implement all algorithmic specifications detailed in Section 5 without degrading the accuracy of any data used in the processing.

ALG-HGH-010-A0

The usage of reference frames shall comply with the definitions expressed in [AD 7] and Appendix C. In the event of conflict, Appendix C takes precedence.

ALG-HGH-015-A0

The Product Generation Function shall provide all the functionality required to support the following:

1. reception and acceptance of the GOME-2 level 0 data stream,
2. reception and acceptance and validation of all other input data required by the processor (e.g. instrument telemetry data, initialisation data, orbit data, static auxiliary data, key data, correction factor data, inflight auxiliary calibration data, other products etc.)
3. processing of data in all earth observation instrument modes,
4. processing of data in all calibration instrument modes,
5. processing of data in all other instrument modes,
6. processing from level 0 to level 1a,
7. processing from level 1a to 1b
8. geolocation processing to level 1a and level 1b, via the PGE service providing common attitude and orbit information,
9. full on-line quality control of the data via a Product Quality Evaluation (PQE) functionality,
10. estimation and update of the time-varying degradation correction factors used in the processing via a Sensor Performance Assessment (SPA) functionality,
11. generation of monitoring and quality information on the observed GOME-2 instrument status and the GOME-2 Level 1 Product Generation Function status via the PGE services and PQE and SPA functionality, monitoring and control interfacing functions using the generic PGE services.
12. monitoring and control interfacing functions using the generic PGE services.

ALG-HGH-020-A0

Each function of the PGF shall monitor its performance and raise events of user-configurable severity on the occurrence of:

1. any abnormal instrument behaviour being detected
2. any occurrence and transition to/from a non-nominal mode of product generation
3. any non-nominal operation of the function
4. any occurrence likely to affect the product quality.

ALG-HGH-025-A0

The Product Generation Function shall support the production of level 1a/1b products in a nominal manner for input data acquired by the following Instruments and Platforms configurations also in parallel:

1. MetOp-1/GOME-2 Instrument
2. MetOp-2/GOME-2 Instrument
3. MetOp-3/GOME-2 Instrument

ALG-HGH-030-A0

The Product Generation Function shall process the level 0 data and produce level 1a and 1b data of a nominal quality for all nominal modes and states of the instrument which shall include the following:

1. Nadir scanning
2. North polar scanning
3. South polar scanning
4. Other scanning
5. Nadir static
6. Other static
7. Dark
8. Sun (over diffuser)
9. White light source (direct)
10. Spectral light source (direct)
11. Spectral light source over diffuser
12. LED
13. Moon
14. Idle
15. Test
16. Dump

ALG-HGH-035-A0

The product generation function shall process the level 0 data and produce level 1a and level 1b data in a non-nominal manner in the following modes and states of the instrument, if applicable:

1. missing, corrupt, or repeated instrument level 0
2. missing, corrupt, or repeated satellite telemetry packets
3. missing, corrupt, or repeated ancillary or auxiliary data

ALG-HGH-040-A0

The Product Generation Function shall process the level 0 data and produce level 1a and level 1b data in a non-nominal manner in the following modes and states of the instrument:

1. continuous operation with missing channels implying reduced spectral coverage
2. continuous operation with reduced swath implying reduced geographical coverage
3. continuous operation with non-nominal pointing

ALG-HGH-045-A0

The GOME-2 Product Generation Function shall support, in nominal operational situation, in addition to the operation of data from the continuous part of a dump the processing before and after data gaps.

ALG-HGH-055-A0

Any coefficient or constant used within the PGF shall be user-configurable.

ALG-HGH-060-A0

Calculation of mean, standard deviation and mean error of detector readouts where required shall be carried out as specified in Section 5.8.1.

ALG-HGH-065-A0

Linear interpolation where required shall be carried out as specified in Section 5.8.2.

ALG-HGH-070-A0

Spline interpolation where required shall be carried out as specified in Section 5.8.3.

ALG-HGH-075-A0

Akima interpolation where required shall be carried out as specified in Section 5.8.4.

4.3 Specific Requirements

4.3.1 Functional Requirements (FCT)

4.3.1.1 Functional Requirements on (A1)

ALG-FCT-004-A1

RECEIVE AND VALIDATE LEVEL 0 AND AUXILIARY DATA (A1)

The Receive and Validate Level 0 and Auxiliary Data (A1) functionality shall perform, in addition to the generic checks identified in the CGSRD [AD 1], the instrument-specific acceptance and checking of the input data as specified in Section 5.1.

ALG-FCT-005-A1.1

RECEIVE & VALIDATE LEVEL 0 DATA FLOW (A1.1)

The Receive & Validate Level 0 Data Flow (A1.1) functionality shall check and validate the level 0 data flow from the GOME-2 instrument as specified in Section 5.1.1.

ALG-FCT-006-A1.2

RECEIVE, VALIDATE AND CORRELATE SIDE INFORMATION (A1.2)

The Receive, Validate & Correlate Side Information (A1.2) functionality shall receive and validate the side information required by the GOME-2 PGF and relate them to the level 0 data flow from the GOME-2 instrument as specified in Section 5.1.2.

ALG-FCT-007-A1.2

RECEIVE, VALIDATE AND CORRELATE SIDE INFORMATION (A1.2)

The Receive, Validate & Correlate Side Information (A1.2) functionality shall compile and format the Level 0 appended information in accordance with [AD 4], using the validated input data.

4.3.1.2 Functional Requirements on (A2)

ALG-FCT-025-A2

LEVEL 0 TO 1A PROCESSING (A2)

The GOME-2 level 0 to 1a processor shall produce level 1a data using algorithms detailed in Section 5.2. The content of the level 1a data and its format shall be as specified in [AD 4] and [AD 5]. ***Note*****:** References to the variables contained within [AD4] and [AD 5] are included in the variable tables of Section 5.2. In the case of conflict, the variable tables of Section 5.2 shall take precedence.

ALG-FCT-026-A2
LEVEL 0 TO 1A PROCESSING (A2) The GOME-2 level 0 to 1a processor shall make available for inspection, both inside and outside the Core Ground Segment, the input and output variables of each algorithmic module specified in Section 5.2as detailed in the variable tables contained therein.

ALG-FCT-027-A2
LEVEL 0 TO 1A PROCESSING (A2) The application of calibration steps to data of all measurements modes, including the provision of a user-configurable selection of calibration steps, shall be carried out as specified in Appendix A.

ALG-FCT-028-A2
LEVEL 0 TO 1A PROCESSING (A2) The order of application of calibration steps to data of all measurement modes shall be carried out as specified in Figure 5, Figure 6, Figure 7, and Figure 8.

ALG-FCT-030-A2.0
READ INPUT DATA (A2.0) The GOME-2 level 0 to 1a processor shall be able to accept and validate the following data as specified in Section via the PGE: 1. initialisation data 2. orbit and time correlation data 3. static auxiliary data 4. pre-flight calibration key data 5. degradation correction factor data 6. in-flight calibration data 7. a level 0 data input stream as specified in [AD4] and [AD5]

ALG-FCT-031-A2.0
READ INPUT DATA (A2.0) The input data to the GOME-2 level 0 to 1a processor shall be configuration controlled.

ALG-FCT-040-A2.0.1
READ INITIALISATION DATA (A2.0.1) At the beginning of a GOME-2 level 0 to 1a processor run the initialisation data as specified in Section 5.2.2.3shall be read.

ALG-FCT-041-A2.0.1

READ INITIALISATION DATA (A2.0.1)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-042-A2.0.2

READ ORBIT AND TIME CORRELATION DATA (A2.0.2)

At the beginning of a GOME-2 level 0 to 1a processor run the orbit data, and if UTC option 3 of Determine UTC Time Grid (A2.3.2) is selected, the time correlation data, as specified in Section 5.2.2.3 shall be read.

ALG-FCT-043-A2.0.2

READ ORBIT AND TIME CORRELATION DATA (A2.0.2)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-044-A2.0.3

READ STATIC AUXILIARY DATA (A2.0.3)

At the beginning of a GOME-2 level 0 to 1a processor run the initialisation data as specified in Section 5.2.2.3 shall be read.

ALG-FCT-045-A2.0.3

READ STATIC AUXILIARY DATA (A2.0.3)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-050-A2.0.4

READ KEY DATA (A2.0.4)

At the beginning of a GOME-2 level 0 to 1a processor run the pre-flight calibration key data as specified in Section 5.2.2.3 shall be read.

ALG-FCT-051-A2.0.4

READ KEY DATA (A2.0.4)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-052-A2.0.5

READ CORRECTION FACTOR DATA (A2.0.5)

At the beginning of a GOME-2 level 0 to 1a processor run the degradation correction factor data as specified in Section 5.2.2.3 shall be read.

ALG-FCT-053-A2.0.5

READ CORRECTION FACTOR DATA (A2.0.5)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded, an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode. If the data are not available, the PGF shall behave in a fashion consistent with no degradation.

ALG-FCT-045-A2.0.6

READ IN-FLIGHT CALIBRATION DATA (A2.0.6)

At the beginning of a GOME-2 level 0 to 1a processor run the in-flight calibration data as specified in Section 5.2.2.3 shall be read.

ALG-FCT-046-A2.0.6

READ IN-FLIGHT CALIBRATION DATA (A2.0.6)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-055-A2.0.7

READ LEVEL 0 INPUT DATA, SEPARATE SCANS AND GENERATE PCDS

(A2.0.7) At the beginning of a GOME-2 level 0 to 1a processor run the level 0 data stream or product as specified in [AD 4] and [AD 9] shall be read.

ALG-FCT-056-A2.0.7

READ LEVEL 0 INPUT DATA, SEPARATE SCANS AND GENERATE PCDS

(A2.0.7) The data stream or product shall be split into individual scans each comprising a maximum of 16 data packets as specified in Section 5.2.2.4 and the global Product Confidence Data records specified in Section 5.2.2.3 shall be calculated.

ALG-FCT-075-A2.1

PREPROCESS MÜLLER MATRIX ELEMENTS (A2.1)

This function shall calculate the Müller Matrix elements (see Appendix E and E.2) from the Calibration Key Data as specified in Section 5.2.3.

ALG-FCT-090-A2.2

CONVERT HOUSEKEEPING DATA (A2.2)

The Product Generation Function shall convert the subset of GOME-2 housekeeping data required for subsequent processing, from the raw instrument binary units into engineering units as specified in Section 5.2.4.

ALG-FCT-085-A2.3

DETERMINE OBSERVATION MODE AND VIEWING ANGLES (A2.3)

The observation mode, and PMD transfer and readout modes for a scan shall be derived from a combination of housekeeping data and the scanner viewing angles as specified in Section 5.2.6.

ALG-FCT-091-A2.4

DETERMINE PCDS FROM RAW INTENSITY (A2.4)

Generic saturation and hot pixel checks shall be applied to the raw intensity as specified in Section 5.2.6.

ALG-FCT-095-A2.5

PREPARE PMD DATA (A2.5)

The PMD band signals shall be reconstructed for PMD band transfer data by multiplying the signals in the Science Data Packet with their respective co-adding factors as specified in Section 5.2.7.

ALG-FCT-100-A2.6

CALCULATE GEOLOCATION FOR FIXED GRID (A2.6)

The geolocation function shall calculate a set of geolocation parameters (depending on the instrument mode) from an orbit state vector containing its own UTC time stamp, the UTC contained time stamp in the Science Data Packet as specified in [AD 9] and scanner viewing angles as specified in Section 5.2.8.

ALG-FCT-105-A2.6.1

DETERMINE SUB-SATELLITE POINT (A2.6.1)

Latitude, longitude, and satellite height shall be calculated on a 187.5 ms grid synchronised with every second scanner position and distances to sun and moon shall be calculated as specified in Section 5.2.8.4.

ALG-FCT-110-A2.6.2

CALCULATE LINE-OF-SIGHT ANGLES FOR THE GROUND FOOTPRINT (A2.6.2)
The LOS elevation and azimuth angles in the Satellite Relative Actual Reference CS shall be derived from the scanner viewing angle and the IFOV dimensions as specified in Section 5.2.8.4. These calculations shall be performed for the Earth observation mode only.

ALG-FCT-115-A2.6.3

CALCULATE TARGET POINTING INFORMATION (A2.6.3)
The target pointing information shall be calculated (depending on instrument mode) as specified in Section 5.2.8.4.

ALG-FCT-116-A2.7

DETERMINE PCDS FROM GEOLOCATION (A2.7)
Generic South Atlantic Anomaly, Sunglint and Rainbow checks are applied to data from all measurement modes as specified in Section 5.2.9.

ALG-FCT-120-A2.8

CALCULATE DARK SIGNAL CORRECTION (A2.8)
Dark signal correction parameters shall be calculated on the basis of all measurements made in *dark* calibration mode, on the dark side of the orbit as specified in Section 5.2.10. **Note:** All scans in one *dark* observation mode period shall be accumulated.

ALG-FCT-125-A2.8

CALCULATE DARK SIGNAL CORRECTION (A2.8)

The newly calculated dark signal correction parameters shall be output to the inflight calibration data storage location.

ALG-FCT-130-A2.9

APPLY DARK SIGNAL CORRECTION (A2.9)

The dark signal correction parameters which have been supplied as in-flight calibration data input to the processor shall be applied and the absolute error on the corrected measurements calculated, as specified in Section 5.2.11.

ALG-FCT-131-A2.10

NORMALISE SIGNALS TO ONE SECOND INTEGRATION TIME (A2.10)

All signals previously corrected for Dark Signal shall be normalised to an effective Integration Time of one second as specified in Section 5.2.12.

ALG-FCT-135-A2.11

CALCULATE PPG (A2.11)

Using data measured in *LED* calibration mode the PPG correction shall be calculated as specified in Section 5.2.13. ***Note*:** All scans in one LED observation mode period shall be accumulated.

ALG-FCT-136-A2.11

CALCULATE PPG (A2.11)

Depending on the setting of a user configurable initialisation parameter the calculation of PPG as specified in Section 5.2.13 shall be carried out using measurements from *WLS* calibration mode. ***Note*:** In this case the algorithm shall remain the same.

ALG-FCT-140-A2.11

CALCULATE PPG (A2.11)

The newly calculated PPG correction parameters shall be output to the in-flight calibration data storage location.

ALG-FCT-145-A2.12

APPLY PPG CORRECTION (A2.12)

The PPG correction parameters which have been supplied as in-flight calibration data input to the processor shall be applied and the absolute error on the corrected measurements calculated, as specified in Section 5.2.14.

ALG-FCT-150-A2.13

CALCULATE SPECTRAL CALIBRATION PARAMETERS FOR MAIN CHANNELS (A2.13)

Using data measured in *SLS* calibration mode the spectral calibration parameters shall be calculated as specified in Section 5.2.15. ***Note*:** All scans in one *SLS* observation mode period shall be accumulated.

ALG-FCT-155-A2.13

CALCULATE SPECTRAL CALIBRATION PARAMETERS FOR MAIN CHANNELS (A2.13)

The newly calculated spectral calibration parameters shall be output to the in-flight calibration data storage location.

ALG-FCT-160-A2.14
CALCULATE SPECTRAL CALIBRATION PARAMETERS FOR PMD CHANNELS (A2.14)
Using data measured in *SLS* calibration mode the spectral calibration parameters of the PMDs shall be calculated as specified in Section 5.2.16. ***Note*****:** All scans in one *SLS* observation mode period shall be accumulated.

ALG-FCT-160-A2.14
CALCULATE SPECTRAL CALIBRATION PARAMETERS FOR PMD CHANNELS (A2.14)
Using data measured in *SLS* calibration mode the spectral calibration parameters of the PMDs shall be calculated as specified in Section 5.2.16. ***Note*****:** All scans in one *SLS* observation mode period shall be accumulated.

ALG-FCT-165-A2.14
CALCULATE SPECTRAL CALIBRATION PARAMETERS FOR PMD CHANNELS (A2.14)
The newly-calculated PMD spectral calibration parameters shall be output to the in-flight calibration data storage location.

ALG-FCT-170-A2.15
APPLY SPECTRAL CALIBRATION PARAMETERS (A2.15)
The spectral calibration parameters which have been supplied as in-flight calibration data input to the processor shall be applied as specified in Section 5.2.17.

ALG-FCT-175-A2.16
CALCULATE ETALON CORRECTION (A2.16)
Using data measured in *WLS* calibration mode, the Etalon parameters shall be calculated as specified in Section 5.2.18. ***Note*****:** All scans in one *WLS* observation mode period shall be accumulated.

ALG-FCT-176-A2.16
CALCULATE ETALON CORRECTION (A2.16)
Depending on the setting of a user configurable initialisation parameter the calculation of Etalon correction as specified in Section 5.2.18 shall be carried out using measurements from *Sun* calibration mode. ***Note***: In this case, the algorithm shall remain the same.

ALG-FCT-180-A2.16

CALCULATE ETALON CORRECTION (A2.16)

The newly calculated Etalon correction parameters shall be output to the in-flight calibration data storage location.

ALG-FCT-185-A2.17

APPLY ETALON CORRECTION (A2.17)

The Etalon correction parameters which have been supplied as in-flight calibration data input to the processor shall be applied and the absolute error on the corrected spectrum calculated, as specified in Section 5.2.19.

ALG-FCT-190-A2.18

DETERMINE STRAYLIGHT CORRECTION (A2.18)

A straylight correction shall be determined for each detector pixel on the basis of the measured intensity and the pre-flight calibration Key data as specified in Section 5.2.20.

ALG-FCT-195-A2.19

APPLY STRAYLIGHT CORRECTION (A2.19)

The straylight correction parameters which have been calculated as specified in Section 5.2.20 shall be applied and the absolute error on the corrected measurement calculated, as specified in Section 5.2.21.

ALG-FCT-200-A2.20

CALCULATE SMR (A2.20)

Using data measured in *Sun* calibration mode a Solar Mean Reference (SMR spectrum shall be calculated as specified in Section 5.2.22. ***Note*****:** All scans in one *Sun* observation mode period shall be accumulated.

ALG-FCT-205-A2.21

DETERMINE STOKES FRACTIONS (A2.21)

The Stokes fractions describing the polarisation state of the incoming light shall be determined as specified in Section 5.2.23.

ALG-FCT-225-A2.22

COLLECT GLOBAL PCDS PER PRODUCT (A2.22)

All of the global PCDs listed in Section 5.2.24.3 shall be collated and passed to Write Level 0 and 1a Product (A2.23) to be formatted in the level 1a product as specified in [AD 4] and [AD 5].

ALG-FCT-035-A2.23
WRITE LEVEL 0 AND 1A PRODUCT (A2.23) The GOME-2 level 0 to 1a processor shall output one level 0 data product in accordance with [AD 4] and [AD 5] covering the same amount of data as the corresponding level 0 data provided on input.

ALG-FCT-036-A2.23
WRITE LEVEL 0 AND 1A PRODUCT (A2.23) The GOME-2 level 0 to 1a processor shall output one level 1a data product in accordance with [AD4] and [AD5] covering the same amount of data as the corresponding level 0 data provided on input.

4.3.1.3 Functional Requirements on (A3)

ALG-FCT-290-A3
LEVEL 1A TO 1B PROCESSING (A3) The GOME-2 level 1a to 1b processor shall produce level 1b data using algorithms detailed in Section 5.3. The content of the level 1b data and its format shall be as specified in [AD 4] and [AD 5]. ***Note*:** References to the variables contained within [AD 4] and [AD 5] are included in the variable tables of Section 5.3. In the case of conflict the variable tables of Section 5.3 shall take precedence.

ALG-FCT-291-A3
LEVEL 1A TO 1B PROCESSING (A3) The GOME-2 level 0 to 1a processor shall make available for inspection, both inside and outside the Core Ground Segment, the input and output variables of each algorithmic module specified in Section 5.3 as detailed in the variable tables contained therein.

ALG-FCT-292-A3
LEVEL 1A TO 1B PROCESSING (A3) The application of calibration steps to data of all measurements modes, including the provision of a user-configurable selection of calibration steps shall be carried out as specified in Appendix A.

ALG-FCT-293-A3
LEVEL 1A TO 1B PROCESSING (A3) The order of application of calibration steps to data of all measurements modes, shall be carried out as specified in Figure 18, Figure 11, Figure 12 and Figure 13.

ALG-FCT-296-A3.0

READ INPUT DATA (A3.0)

The GOME-2 level 1a to 1b processor shall be able to accept and validate the following data as specified in Section 5.3.2 via the PGE:

1. initialisation data
2. static auxiliary data
3. pre-flight calibration key data
4. a level 1a data input stream as specified in [AD 4] and [AD 5].

ALG-FCT-297-A3.0

READ INPUT DATA (A3.0)

The input data to the GOME-2 level 0 to 1a processor shall be configuration controlled.

ALG-FCT-298-A3.0.1

READ INITIALISATION DATA (A3.0.1)

At the beginning of a GOME-2 level 1a to 1b processor run the initialisation data as specified in Section 5.3.2.3 shall be read.

ALG-FCT-299-A3.0.1

READ INITIALISATION DATA (A3.0.1)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-301-A3.0.2

READ STATIC AUXILIARY DATA (A3.0.2)

At the beginning of a GOME-2 level 1a to 1b processor run the static auxiliary data as specified in Section 5.3.2.3 shall be read.

ALG-FCT-302-A3.0.2

READ STATIC AUXILIARY DATA (A3.0.2)

The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-303-A3.0.3
READ KEY DATA (A3.0.3) At the beginning of a GOME-2 level 1a to 1b processor run the pre-flight calibration key data as specified in Section 5.3.2.3 shall be read.

ALG-FCT-304-A3.0.3
READ KEY DATA (A3.0.3) The data specified shall be compared against user-configurable boundaries and in the event that these boundaries are exceeded an event of user-configurable severity shall be sent via the PGE and processing shall continue in degraded mode.

ALG-FCT-305-A3.0.4
READ LEVEL 1A INPUT DATA (A3.0.4) At the beginning of a GOME-2 level 1a to 1b processor run the level 1a data stream or product as specified in [AD 4] and [AD 9] shall be read.

ALG-FCT-306-A3.0.4
READ LEVEL 1A INPUT DATA (A3.0.4) The data stream or product shall be separated into individual scans as specified in Section 5.3.2.4.

ALG-FCT-310-A3.1
PREPARE PMD DATA (A3.1) The PMD band signals shall be reconstructed for PMD band transfer data by multiplying the signals in the Science Data Packet with their respective co-adding factors as specified in Section 5.3.3.

ALG-FCT-311-A3.2
CALCULATE GEOLOCATION FOR ACTUAL INTEGRATION TIMES (A3.2) The geolocation information shall be calculated for each specific integration time from the geolocation information of the fixed grid as specified in Section 5.3.4.

ALG-FCT-315-A3.3
APPLY DARK SIGNAL CORRECTION (A3.3) The dark signal correction parameters which have been supplied in the VIADRs of the level 1a product or data stream shall be applied and the absolute error on the corrected measurements calculated, as specified in Section 5.3.5.

ALG-FCT-316-A3.4
NORMALISE SIGNALS TO ONE SECOND INTEGRATION TIME (A3.4)
All signals previously corrected for Dark Signal shall be normalised to an effective Integration Time of one second as specified in Section 5.3.6

ALG-FCT-320-A3.5
APPLY PPG CORRECTION (A3.5)
The PPG correction parameters which have been supplied in the VIADRs of the level 1a product or data stream shall be applied and the absolute error on the corrected measurements calculated, as specified in Section 5.3.7.

ALG-FCT-325-A3.6
APPLY SPECTRAL CALIBRATION PARAMETERS (A3.6)
The spectral calibration parameters which have been supplied in the VIADRs of the level 1a product or data stream shall be applied and the absolute error on the corrected measurements calculated, as specified in Section 5.3.8.

ALG-FCT-330-A3.7
APPLY ETALON CORRECTION (A3.7)
The spectral calibration parameters which have been supplied in the VIADRs of the level 1a product or data stream shall be applied and the absolute error on the corrected measurements calculated, as specified in Section 5.3.9.

ALG-FCT-335-A3.8
DETERMINE STRAYLIGHT CORRECTION (A3.8)
A straylight correction shall be determined for each detector pixel on the basis of the measured intensity and the pre-flight calibration Key data as specified in Section 5.3.10.

ALG-FCT-340-A3.9
APPLY STRAYLIGHT CORRECTION (A3.9)
The straylight correction parameters which have been calculated as specified in Section 5.3.10 shall be applied and the absolute error on the corrected measurement calculated, as specified in Section 5.3.11.

ALG-FCT-345-A3.10
APPLY POLARISATION CORRECTION (A3.10)
The stokes fractions which have been supplied in the MDRs of the level 1a data product or data stream shall be applied to correct for the polarisation state of the incoming radiation and the absolute error on the corrected measurement calculated, as specified in Section 5.3.12.

ALG-FCT-360-A3.11

APPLY RADIANCE RESPONSE (A3.11)

The measured data shall be corrected for the radiance response of the instrument as specified in Section 5.3.13.

ALG-FCT-361-A3.12

APPLY IRRADIANCE RESPONSE (A3.12)

The data measured in *Sun* calibration mode shall be corrected for the irradiance response of the instrument as specified in Section 5.3.14.

ALG-FCT-361-A3.13

CORRECT DOPPLER SHIFT (A3.13)

The data measured in *Sun* calibration mode shall be corrected for the Doppler shift due to the motion of the satellite of the instrument as specified in Section 5.3.15.

ALG-FCT-365-A3.14

REDUCE SPATIAL ALIASING (A3.14)

The effect due the finite detector pixel readout time which causes individual detector pixels to view slightly shifted ground scenes, referred to as ‘Spatial Aliasing’, shall be corrected using the algorithm specified in Section 5.2.16.

ALG-FCT-220-A3.15

CALCULATE FRACTIONAL CLOUD COVER AND CLOUD TOP PRESSURE (A3.15)

An effective fractional cloud cover and cloud top pressure shall be determined for each GOME-2 ground pixel using main channel detector readouts from in and around the Oxygen-A band as described in Section 5.3.17.

ALG-FCT-366-A3.16

COLLECT GLOBAL PCDS PER PRODUCT (A3.16)

All of the global PCDs listed in Section 5.3.18.8.3 shall be collated and passed to Write Level 1b Product (A3.17) to be formatted in the level 1a product as specified in [AD 4] and [AD 5].

ALG-FCT-370-A3.17

WRITE LEVEL 1B PRODUCT (A3.17)

The GOME-2 level 1a to 1b processor shall output one level 1a data product in accordance with [AD 4] and [AD 5] covering the same amount of data as the corresponding level 0 data provided on input.

4.3.1.4 Functional Requirements on (A4)

ALG-FCT-375-A4

SENSOR PERFORMANCE ASSESSMENT (SPA) (A4)

The Sensor Performance Assessment (SPA) functionality shall generate monitoring information, for monitoring in-flight instrument performance for the lifetime of the mission, comprising selected housekeeping data, selected spectral data, and in-flight calibration data as specified in Section 5.4.

ALG-FCT-376-A4

SENSOR PERFORMANCE ASSESSMENT (SPA) (A4)

The monitoring information generated by the SPA functionality shall be stored for the lifetime of the mission in the SPA data storage location.

ALG-FCT-377-A4

SENSOR PERFORMANCE ASSESSMENT (SPA) (A4)

The SPA functionality shall generate degradation correction factors from the monitoring information as specified as in Section 5.4.

ALG-FCT-378-A4

SENSOR PERFORMANCE ASSESSMENT (SPA) (A4)

The degradation correction factors generated by the SPA functionality shall be under configuration control.

ALG-FCT-379-A4

SENSOR PERFORMANCE ASSESSMENT (SPA) (A4)

The monitoring information and degradation correction factors generated by the SPA functionality shall be made available to Visualisation (A6).

ALG-FCT-380-A4.1

SPA EXTRACTION AND PRE-PROCESSING (A4.1)

The SPA extraction and pre-processing functionality shall be able to accept and validate the following data as specified in Section 5.4 via the PGE:

1. initialisation data
2. level 1a data product or stream as specified in [AD4] and [AD5]
3. level 1b data product or stream as specified in [AD4] and [AD5]
4. in-flight calibration data from the in-flight calibration data storage location

ALG-FCT-381-A4.1
SPA EXTRACTION AND PRE-PROCESSING (A4.1)
The monitoring data shall be extracted from level 1a products, level 1b products, and in-flight calibration data files, preprocessed and written to the SPA data storage location as specified in Section 5.4.2.3.

ALG-FCT-405-A4.2
SPA ANALYSIS (A4.2)
The SPA analysis functionality specified in specified in Section 5.4.3.4 shall be made available to an operator via a manual interface for the determination of degradation correction factors and condensed monitoring information.

ALG-FCT-420-A4.2
SPA ANALYSIS (A4.2)
The SPA data storage location shall be made available to an operator via a manual interface for the determination of degradation correction factors and condensed monitoring information.

4.3.1.5 Functional Requirements on (A5)

ALG-FCT-425-A5
PRODUCT QUALITY EVALUATION (A5)
The Product Quality Evaluation (PQE) functionality shall provide information about the quality of the generated level 1a and level 1b data products as specified in Section 5.5.

ALG-FCT-426-A5
PRODUCT QUALITY EVALUATION (A5)
The quality information generated by the PQE functionality shall be stored for the lifetime of the mission in the PQE data storage location.

ALG-FCT-427-A5
PRODUCT QUALITY EVALUATION (A5)
The quality information generated by the PQE functionality shall be made available to Visualisation (A6).

ALG-FCT-428-A5.1
PQE EXTRACTION (A5.1) The PQE extraction functionality shall be able to accept and validate the following data as specified in Section 5.5 via the PGE: 1. initialisation data 2. level 1a data product as specified in [AD4] and [AD5] 3. level 1b data product as specified in [AD4] and [AD5]

ALG-FCT-430-A5.1
PQE EXTRACTION (A5.1) The PQE Extraction functionality shall extract all data specified in Section 5.5.2.3 make it available to Process Product Quality Information (A5.2).

ALG-FCT-431-A5.1
PQE EXTRACTION (A5.1) The PQE data storage location shall be updated with all data extracted by PQE Extraction (A5.1) as specified in Section 5.5.2.3.

ALG-FCT-445-A5.2
PROCESS PRODUCT QUALITY INFORMATION (A5.2) The data extracted by PQE Extraction (A5.1) are further condensed to provide daily, weekly, monthly and yearly Product Quality Summaries, and daily "Quick-Look" products as specified in Section 5.5.3.4.

ALG-FCT-447-A5.2
PROCESS PRODUCT QUALITY INFORMATION (A5.2) The PQE data storage location shall be updated with all Product Quality summaries and "Quick Look" products generated by Process Product Quality Information (A5.2).

4.3.1.6 Functional Requirements on (A6)

ALG-FCT-461-A6
VISUALISATION (A6) The dataset to be visualised and the type of visualisation to be performed shall be user selectable.

ALG-FCT-465-A6
VISUALISATION (A6) An HMI shall be available for control of the visualisation functionality.

ALG-FCT-470-A6
VISUALISATION (A6)
The visualisation tool shall accept GOME-2 Science Data Packets as input.

ALG-FCT-475-A6
VISUALISATION (A6)
The visualisation tool shall accept level 0 products as input

ALG-FCT-480-A6
VISUALISATION (A6)
The visualisation tool shall accept level 1a products as input

ALG-FCT-485-A6
VISUALISATION (A6)
The visualisation tool shall accept level 1b products as input

ALG-FCT-490-A6
VISUALISATION (A6)
The visualisation tool shall accept in-flight calibration data as input.

ALG-FCT-495-A6
VISUALISATION (A6)
The visualisation tool shall accept monitoring information and corrections factors produced by the SPA functionality as input.

ALG-FCT-500-A6
VISUALISATION (A6)
The visualisation tool shall accept the quality information produced by the PQE functionality as input.

ALG-FCT-505-A6
VISUALISATION (A6)
The user shall be able to select via the HMI the type of product to be displayed e.g. SDP, level 0 product, level 1 product, level 1b product, in-flight calibration data, correction factors, monitoring information or quality information.

ALG-FCT-510-A6
VISUALISATION (A6)
The user shall be able to select via the HMI one or more datasets or products of the selected type to be displayed.

ALG-FCT-515-A6
VISUALISATION (A6)
The visualisation tool shall display the headers of the loaded files in ASCII format on user's request.

ALG-FCT-520-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 0 data via the time series visualisation functionality.

ALG-FCT-525-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 0 data via the spectra visualisation functionality.

ALG-FCT-530-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 1a data via the time series visualisation functionality.

ALG-FCT-535-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 1a data via the spectra visualisation functionality.

ALG-FCT-540-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 1a data via the map visualisation functionality.

ALG-FCT-545-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 1b data via the time series visualisation functionality.

ALG-FCT-550-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 1b data via the spectra visualisation functionality.

ALG-FCT-555-A6.1
SDP, LEVEL 0, 1A AND 1B PRODUCT VISUALISATION (A6.1)
It shall be possible to display level 1b data via the map visualisation functionality.

ALG-FCT-560-A6.2
IN-FLIGHT CALIBRATION DATA VISUALISATION (A6.2)
It shall be possible to display in-flight calibration data via the time series visualisation functionality.

ALG-FCT-565-A6.2
IN-FLIGHT CALIBRATION DATA VISUALISATION (A6.2)
It shall be possible to display in-flight calibration data via the spectra visualisation functionality.

ALG-FCT-570-A6.2
IN-FLIGHT CALIBRATION DATA VISUALISATION (A6.2)
It shall be possible to examine individual parameters from the in-flight calibration data.

ALG-FCT-575-A6.3
SPA AND PQE VISUALISATION (A6.3)
It shall be possible to display monitoring information via the time series visualisation functionality.

ALG-FCT-580-A6.3
SPA AND PQE VISUALISATION (A6.3)
It shall be possible to display monitoring information via the spectra visualisation functionality.

ALG-FCT-585-A6.3
SPA AND PQE VISUALISATION (A6.3)
It shall be possible to display monitoring information via the map visualisation functionality.

ALG-FCT-590-A6.3
SPA AND PQE VISUALISATION (A6.3)
It shall be possible to display correction factors via the time series visualisation functionality.

ALG-FCT-595-A6.3
SPA AND PQE VISUALISATION (A6.3)
It shall be possible to display correction factors via the spectra visualisation functionality.

ALG-FCT-600-A6.3
SPA AND PQE VISUALISATION (A6.3)
It shall be possible to display quality information via the time series visualisation functionality.

ALG-FCT-605-A6.3
SPA AND PQE VISUALISATION (A6.3)
It shall be possible to display quality information via the map visualisation functionality.

ALG-FCT-610-A6.1.1
TIME SERIES VISUALISATION (A6.1.1)
The user shall be able to select via a menu provided by the HMI the word or parameter from the selected datasets to be displayed including housekeeping data and selected PMD or FPA pixel detectors.

ALG-FCT-615-A6.1.1
TIME SERIES VISUALISATION (A6.1.1)
The simultaneous display of the same time series for different products or data sets shall be possible with all time series displayed simultaneously on the same plot.

ALG-FCT-620-A6.1.1
TIME SERIES VISUALISATION (A6.1.1)
Different colours shall be used distinguish multiple datasets on the same plot.

ALG-FCT-625-A6.1.1
TIME SERIES VISUALISATION (A6.1.1)
A paging facility shall be provided in order to step through different words or parameters in the selected datasets.

ALG-FCT-630-A6.1.1
TIME SERIES VISUALISATION (A6.1.1)
Statistics of a user selectable subset of the data displayed as a time-series shall be provided comprising minimum, maximum, channel mean and standard deviation.

ALG-FCT-635-A6.1.1
TIME SERIES VISUALISATION (A6.1.1)
The observation mode of the data being displayed shall be indicated as an annotation on the screen.

ALG-FCT-640-A6.1.1

TIME SERIES VISUALISATION (A6.1.1)

There shall be an interactive functionality that allows the user to inspect the values corresponding to the different datasets displayed.

ALG-FCT-645-A6.1.1

TIME SERIES VISUALISATION (A6.1.1)

Additional information (including at a minimum scan sequence number, geolocation information, time of observation, observation mode, pmd transfer and readout modes, on-board lamp currents and voltages and detector bench temperatures) shall be presented to the user for each record under inspection.

ALG-FCT-650-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

The user shall be able to, via the HMI, select and visualise all FPA and PMD channels for a single readout or spectrum.

ALG-FCT-655-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

All six PMD and FPA channels for a single readout or spectrum shall be displayed simultaneously in separate plots.

ALG-FCT-660-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

The simultaneous display of the same spectra for different products or data sets shall be possible with all spectra displayed simultaneously on the same plot.

ALG-FCT-665-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

Different colours shall be used distinguish multiple datasets on the same plot.

ALG-FCT-670-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

A paging facility shall be provided in order to step through sequential readouts or spectra in the selected product or dataset. **Note:** In the case of SDP’s this includes the capability to step through sequential SDP’s.

ALG-FCT-675-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

Statistics of a user selectable subset of the data displayed as a spectrum shall be provided comprising minimum, maximum, channel mean and standard deviation.

ALG-FCT-680-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

The observation mode of the spectra being displayed shall be indicated as an annotation on the screen.

ALG-FCT-685-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

There shall be an interactive functionality that allows the user to inspect the values corresponding to the different spectra displayed.

ALG-FCT-690-A6.1.2

SPECTRA VISUALISATION (A6.1.2)

Additional information (including at a minimum scan sequence number, geolocation information, time of observation, observation mode, pmd transfer and readout modes, on-board lamp currents and voltages and detector bench temperatures) shall be presented to the user for each record under inspection.

ALG-FCT-695-A6.1.3

MAP VISUALISATION (A6.1.3)

Map visualisation shall comprise two maps with different scales presented simultaneously on the same display.

ALG-FCT-700-A6.1.3

MAP VISUALISATION (A6.1.3)

The first component of the map visualisation shall be a global map displaying the sub-satellite location associated with the data being displayed. **Note:** This displays the satellite orbit and geolocation of individual scans.

ALG-FCT-705-A6.1.3

MAP VISUALISATION (A6.1.3)

The second component of the map visualisation shall be a higher geographical resolution map displaying a colour-coded value of the selected parameter using the precise geolocation of each readout.

ALG-FCT-710-A6.1.3

MAP VISUALISATION (A6.1.3)

A legend shall be provided indicating the value of the selected parameter associated with each colour used in the display.

ALG-FCT-715-A6.1.3
MAP VISUALISATION (A6.1.3) The map visualisation functionality shall be available only for geolocated products.

ALG-FCT-720-A6.1.3
MAP VISUALISATION (A6.1.3) The observation mode of the parameter being displayed shall be indicated as an annotation on the screen.

ALG-FCT-725-A6.1.3
MAP VISUALISATION (A6.1.3) There shall be an interactive functionality that allows the user to inspect the values corresponding to the parameter displayed on the map.

ALG-FCT-730-A6.1.3
MAP VISUALISATION (A6.1.3) Additional information (including at a minimum scan sequence number, geolocation information, time of observation, observation mode, pmd transfer and readout modes, on-board lamp currents and voltages and detector bench temperatures) shall be presented to the user for each record under inspection.

4.3.2 Interface Requirements (INT)

ALG-INT-024-A2.0.1
READ INITIALISATION DATA (A2.0.1) All initialisation data required for GOME-2 level 0 to 1a processing as specified in Section 5.2.2 shall be provided via the PGE.

ALG-INT-025-A2.0.2
READ ORBIT AND TIME CORRELATION DATA (A2.0.2) All orbit and time correlation data required for GOME-2 level 0 to 1a processing as specified in Section 5.2.2 shall be provided via the PGE.

ALG-INT-028-A2.0.3
READ STATIC AUXILIARY DATA (A2.0.3) All pre-flight static auxiliary data required for GOME-2 level 0 to 1a processing as specified in Section 5.2.2 shall be provided via the PGE.

ALG-INT-026-A2.0.4
READ KEY DATA (A2.0.4) All pre-flight calibration key data required for GOME-2 level 0 to 1a processing as specified in Section 5.2.2 shall be provided via the PGE.

ALG-INT-027-A2.0.5
READ CORRECTION FACTOR DATA (A2.0.5) All correction factor data required for GOME-2 level 0 to 1a processing as specified in Section 5.2.2 shall be provided via the PGE.

ALG-INT-030-A2.0.6
READ IN-FLIGHT CALIBRATION DATA (A2.0.6) All in-flight calibration parameters required for GOME-2 level 0 to 1a processing as specified in Section 5.2.2 shall be provided via the PGE.

ALG-INT-031-A3.0.1
READ INITIALISATION DATA (A3.0.1) All initialisation data required for GOME-2 level 1a to 1b processing as specified in Section 5.3.2 shall be provided via the PGE.

ALG-INT-032-A3.0.2
READ STATIC AUXILIARY DATA (A3.0.2) All static auxiliary data required for GOME-2 level 1a to 1b processing as specified in Section 5.3.2 shall be provided via the PGE.

ALG-INT-033-A3.0.3
READ KEY DATA (A3.0.3) All pre-flight calibration key data required for GOME-2 level 1a to 1b processing as specified in Section 5.3.2 shall be provided via the PGE.

ALG-INT-035-A2
IN-FLIGHT CALIBRATION PARAMETERS ON INPUT All in-flight calibration parameter data generated will be stored in the in-flight calibration data storage location and shall be capable of being made available on demand to the processing function via the PGE.

4.3.3 Operational Requirements (OPE)

ALG-OPE-010-A2
MISSING AUXILIARY DATA   If auxiliary data is missing or contains errors, the last valid auxiliary data shall be used and a report of all missing or erroneous auxiliary data and an event of user-configurable severity shall be raised through the EPS reporting service.

ALG-OPE-015-A2
ORBIT STATE VECTOR AND TIME CORRELATION   The product shall be processed using a single set of orbit state vectors and time correlation reference to insure coherency and continuity of orbit and time data within a product.

5 SUPPORTING SCIENCE

In the following sections, functionality defined in the GOME-2 PGS will be specified in detail.

For each algorithmic module the specification will include:

- Table of instrument modes and instrument data to which the module is applicable.
- Listing of subsidiary functions used.
- Objective.
- Description.
- Table of variables.
- Algorithms.

In the variable tables the *Type* indication will follow the notation described below:

enum	enumerated (one byte). Meaning associated with specific values and symbolic names used for these values are given in [AD4] and [AD5].
bool	boolean (one byte). We use 0 for *false* and 1 for *true* throughout. [AD4] allows any non-zero value for *true*, we are more specific here.
b	byte (assume unsigned unless specified otherwise)
w	word (2-byte) (assume unsigned unless specified otherwise)
i	integer (4-byte) (assume **signed** unless specified otherwise)
d	double (8-byte)

To ensure portability between computer systems, [AD4] does not allow data of type float and double in the products. This means any variable of type double will have to be converted to a integer variable before being written to the product. See [AD5] for details: signed or unsigned integer, fixed or variable scaling factor, scaling factor in case a fixed one is used. Furthermore, irrespective of the data type specified for processing of date/time variables within this document they must be converted to *short cds time* as specified in [AD4] and [AD5] before being written to the product.

Sometimes output variables have to be set to “undefined” (e.g., if they cannot be calculated because of missing input variables). [AD4] defines how to represent “undefined” values externally in the products. It is suggested to use *negative infinity* as the internal representation for “undefined” variables of type float (double).

In addition, in all the following algorithm specifications, when interpolation is specified this excludes extrapolation unless explicitly stated.

For the level 1a and 1b products, the number of detector readouts per scan stored in the products shall always equal the number of integration time intervals per scan (6 second / integration time). Readouts with integration time status "aborted" or "forced" are therefore stored only if they would coincide with a "completed" readout for the actual integration time in a scan. For "aborted" and "forced" readouts, the raw values from the science data packet are stored in the level 1a product, and "invalid" values in the level 1b product. Detector signals with integration time status "not completed" are never stored in level 1 products.

The I/O (Input/output) indication will follow the notation described below:

i	Input to the module
o	Output from the module.
t	Temporary use within the module
g	Global to be retained in memory for processing of one complete product assumed to be "dump to dump"

The *Source/Destination* indication will follow the notation described below:

ini	Initialisation dataset	ifc	In-flight calibration dataset
orb	Orbit or time correlation dataset	lv0	Level 0 data stream
stat	Static auxiliary dataset	lv1a	Level 1a data stream
key	Key dataset	lv1b	Level 1b data stream
corr	Correction factor dataset	A.xxx	Algorithmic module A.xxx

Furthermore, unless indicated otherwise:

- Symbol *i* is the detector pixel/PMD band index.
- Symbol *j* is the channel/band index. Enumerated values for channel and band numbers are given in [AD5]. Array variables having channel/band as a dimension shall use the order of channel/bands as defined by these enumerated values.
- Symbol *p* is the value of *j* which indicates PMD p. Symbol *s* is the value of *j* which indicates PMD s. See list of enumerated variables in [AD5] for the actual values.
- Symbol D is the number of detector pixels/PMD bands per channel/band.
- Symbol B is the number of channel/bands. When no distinction between bands within a channel is required this will be 6 (4 FPA + 2 PMD channels). When a distinction is required this will be indicated and the total number of bands is 10 (6 FPA bands, blocks CDE of 2 PMD channels, block B of 2 PMD channels). Symbol B_{FPA} refers specifically to the number of channel/bands in the main FPA channels and BPMD refers to the number of PMD channels.
- Symbol RFPA refers to the number of 187.5 ms integration time ground pixels per 6 s scan: $R_{FPA} = 32$.
- Symbol Rψ refers to the number of scan mirror positions (given every 93.75 ms) per 6 s scan, $R_{\psi} = 64$.
- Symbol RPMD refers to the number of 23.4375 ms integration time PMD ground pixels per 6 s scan: $R_{PMD} = 256$.

5.1 Receive and Validate Level 0 and Auxiliary Data (A1)

In addition to the generic checks identified in the CGSRD [AD1] the functionality that performs the instrument-specific acceptance and checking of the input data is required. Its purpose is to accept the level 0 data, check their integrity, and to perform all checks required for validation of the input data before passing them to the algorithmic functions.

5.1.1 Receive and Validate Level 0 Data Flow (A1.1)

This functionality encompasses the check and validation of the level 0 data flow from the instrument. The generic checks identified in [AD1] are followed by the verification against the expected instrument/SC configuration. The GOME-2 level 0 data flow is checked in three steps, of which the first two are related to the integrity of individual packets, and the last one to the integrity of the sequence of packets.

1. GOME-2 data packets are identified in the data flow via their fixed fields. The length of the data packets is checked.
2. For each packet, the checksum is recalculated and compared against the checksum contained in the packet.
3. A basic check for duplicate packets and the time order of the packets is performed.

Note: The following additional basic checks on level 0 data integrity are part of the to the level 0 to 1a processing:

- A check for missing packets and scans is performed in module Read Level 0 Input Data, Separate Scans and Generate PCDs (A2.0.7).
- The consistency of instrument subsystem settings and the scanner positions are implicitly checked in module Determine Observation Mode and Viewing Angles (A2.3).
- The UTC time stamp is checked in module Determine Observation Mode and Viewing Angles.

5.1.1.1 Identify Data Packets and Check Fixed Fields (A1.1.1)

The GOME-2 Science Data Packet contains a number of fixed fields [AD9]. They shall be used here to identify the individual GOME-2 data packets in the continuous level 0 data flow and to verify their integrity. The following fixed fields shall be used to identify the GOME-2 packets(see [AD9] for their position within the data packet):

- Packet identifier (Packet Primary Header)
- Packet length (Packet Primary Header)
- Length of Ancillary Data
- Fixed Fields 1 to 4 (“GG OO MM EE”)

A packet shall be considered identified if all these fields together are found at the expected position. If no packets can be identified within the level 0 data flow, data are either severely corrupted GOME-2 data or not GOME-2 data at all, and processing cannot continue.

The number of words *N* from one packet identifier to the next one shall be compared to the expected packet length (9369 words). A report shall be raised via the MCS in case a discrepancy is found. If N is found to be smaller than the expected length, the packet is truncated and cannot be processed further. If N is found to be greater than the expected length, only the first 9369 words starting from the packet identifier are considered to constitute the packet. Once a packet is identified, the following additional fields shall be compared to their expected values, and a report shall be raised via the MCS in case a discrepancy is found:

- GOME model (FM 1–3)
- PMD short wavelength indicator
- PMD readout indicator
- 4 × 2 FPA readout indicators

Note: The PMD and FPA readout indicators are constructed from a combination of fixed bits, the subset counter, and part of the packet sequence counter.

5.1.1.2 Check Cyclic Redundancy Code Checksum (A1.1.2)

For each packet identified in A1.1.1, the cyclic redundancy code (CRC) checksum over the complete packet with the exception of the CRC (the last word of the packet) shall be recalculated using a modified CCITT 16-bit checksum (represented by the polynomial $x^{16} + x^{12} + x^5 = 1$).The modification consists of using x0000 as the initial value instead of xFFFF as for the standard check sum. It shall be compared to the CRC in the packet. In case a discrepancy is found, the packet shall be flagged as corrupted and a report shall be raised via the MCS. Corrupted packets shall be written to the level 0 product, but not further processed.

5.1.1.3 Check Packet Sequence Control (A1.1.3)

The packet sequence control is a 14-bit counter which is incremented by 1 in each data packet, and wraps around to 0 when it has reached 2^{14}–1, every 6144 s, or slightly less than once per orbit. It shall be used as a basic check (on all uncorrupted packets) for the following:

- missing packets,
- duplicate packets (this shall be verified by comparing the contents of the two packets with the same packet sequence control),
- packets in the wrong temporal sequence.

In case any of these events is found, a report shall be raised via the MCS. Note that the number of missing packets which shall trigger a report via the MCS shall be user-configurable. In case of duplicate data only the latest data shall be kept.

5.1.2 Receive, Validate and Correlate Side Information (A1.2)

This functionality receives the side-information, validates them and relates them to the level 0 dataflow. It shall be checked that all input data which are needed besides the level 0 data flow (see section 5.2.1 for a list) are available. In case any of them is missing, a report shall be raised via the MCS, and the processing cannot continue. In case some of the in-flight calibration data selected are older than a specified threshold that shall be user configurable, a report shall be raised via the MCS. The processing shall continue using these data and the products shall be flagged as degraded using the fields DEGRADED_PROC_MDR and PCD_BASIC F_OLD_CAL_DATA in the level 1a and 1b products as specified in [AD5]. In case more than one of the in-flight calibration data are older than a specified threshold, the relevant enumerated values detailed in [AD5] shall be added. The checks on the individual input data are not performed here, but after they have been read (A2.0).

5.2 Level 0 to 1a Processing (A2)

5.2.1 Processing Overview

Figures 5, 5a, 5b, 5c show the second level of decomposition for the functional box A2. They provide an overview of required interfaces and the processing flow. The following description concentrates on the input and output data. The processor receives the following input data:

5.2.1.1 Initialisation data

This data set contains all parameter settings for the PGF, such as threshold values, switches between algorithm options, and instrument parameters not contained in the instrument key data.

5.2.1.2 Orbit and Time Correlation Data

For Near Real Time processing a predicted orbit state vector is required as input for the geolocation calculations. During re-processing restituted orbit data are expected to be available. Time correlation information for the calculation of the UTC time grid are provided as external parameters if required by selection of Determine UTC Time Grid, Option 3.

5.2.1.3 Static Auxiliary Data

The static auxiliary data comprises the static databases that are required for use in the level 0 to 1a processor. They are required in particular during the calculation of geolocation information on a fixed grid and the check for sunglint.

5.2.1.4 Key Data

The Key data comprises the complete set of pre-flight calibration data which is provided by the instrument provider.

5.2.1.5 Correction Factor Data

Instrument characteristics such as radiance and irradiance sensitivity will change during the GOME-2 lifetime due to in-orbit degradation of the instrument. Correction factors will be derived in the SPA module (see below) using in-flight measurements and will be made available to the PGF. These correction factors will be set to a default value of “one” representing no degradation at the beginning of the in-orbit life of GOME-2.

5.2.1.6 In-flight Calibration Data

The level 0 to 1a processing includes the determination of in-flight calibration parameters. From measurements of the various calibration sources encountered during each run of the processor, new calibration constants are calculated and written into an in-flight calibration data storage location. They are also retained in memory for use in processing those data acquired after the satellite comes out of the dark side of the orbit and before the next dump. Calibration parameter usage will be updated at the terminator. The terminator is defined by a solar zenith angle in the Northern hemisphere supplied as part of the initialisation dataset. The solar zenith angle will be decreasing as the satellite approaches the terminator. Calibration parameters are expected to be stored for the lifetime of the mission. The calibration constant determination comprises dark current correction, pixel-to-pixel gain correction, determination of spectral calibration parameters, etalon correction, and determination of stray light correction factors for the polarisation and sun measurements.

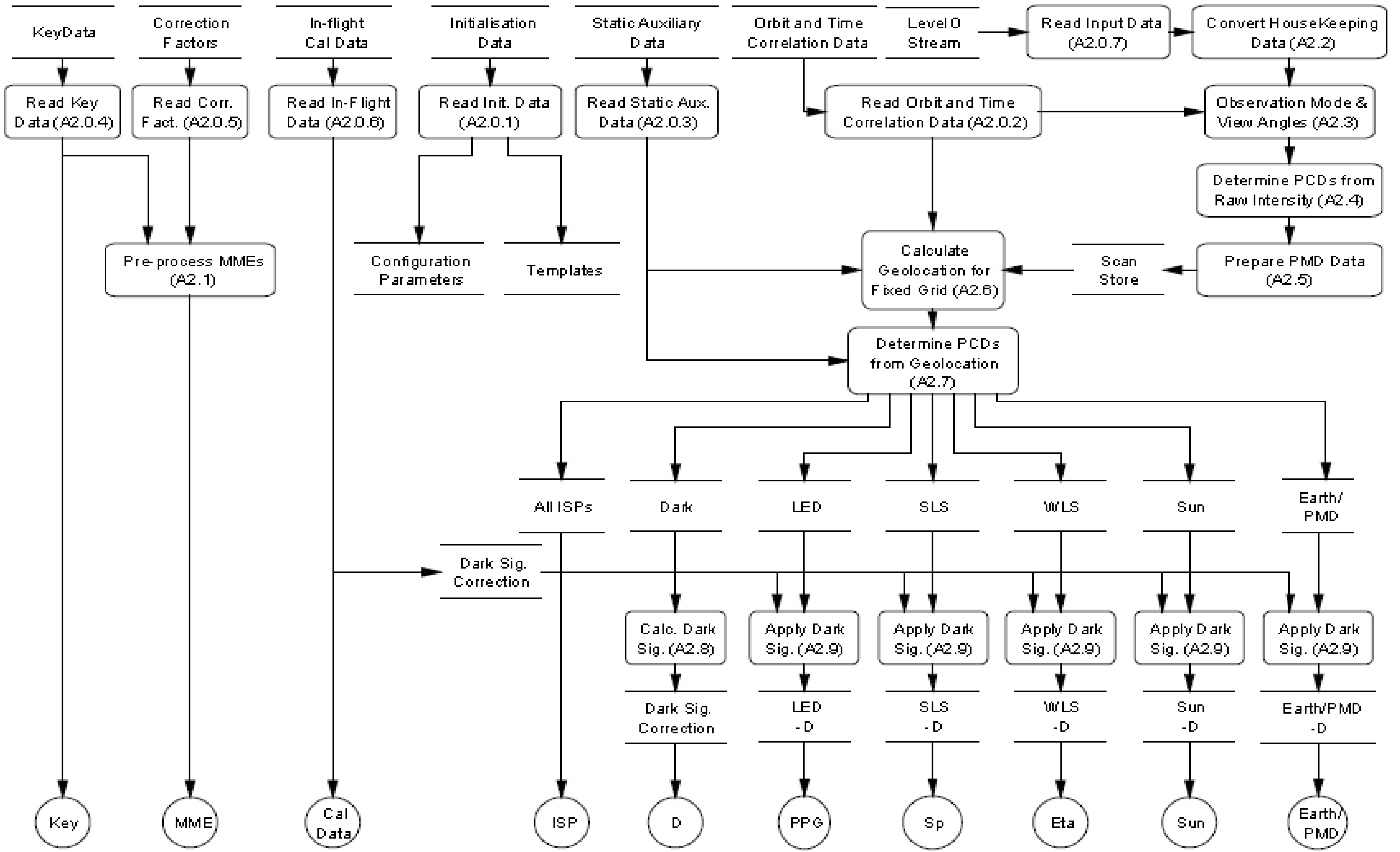

Figure 5: A2 Functional Decomposition: Level 0 to 1a Processor (1).

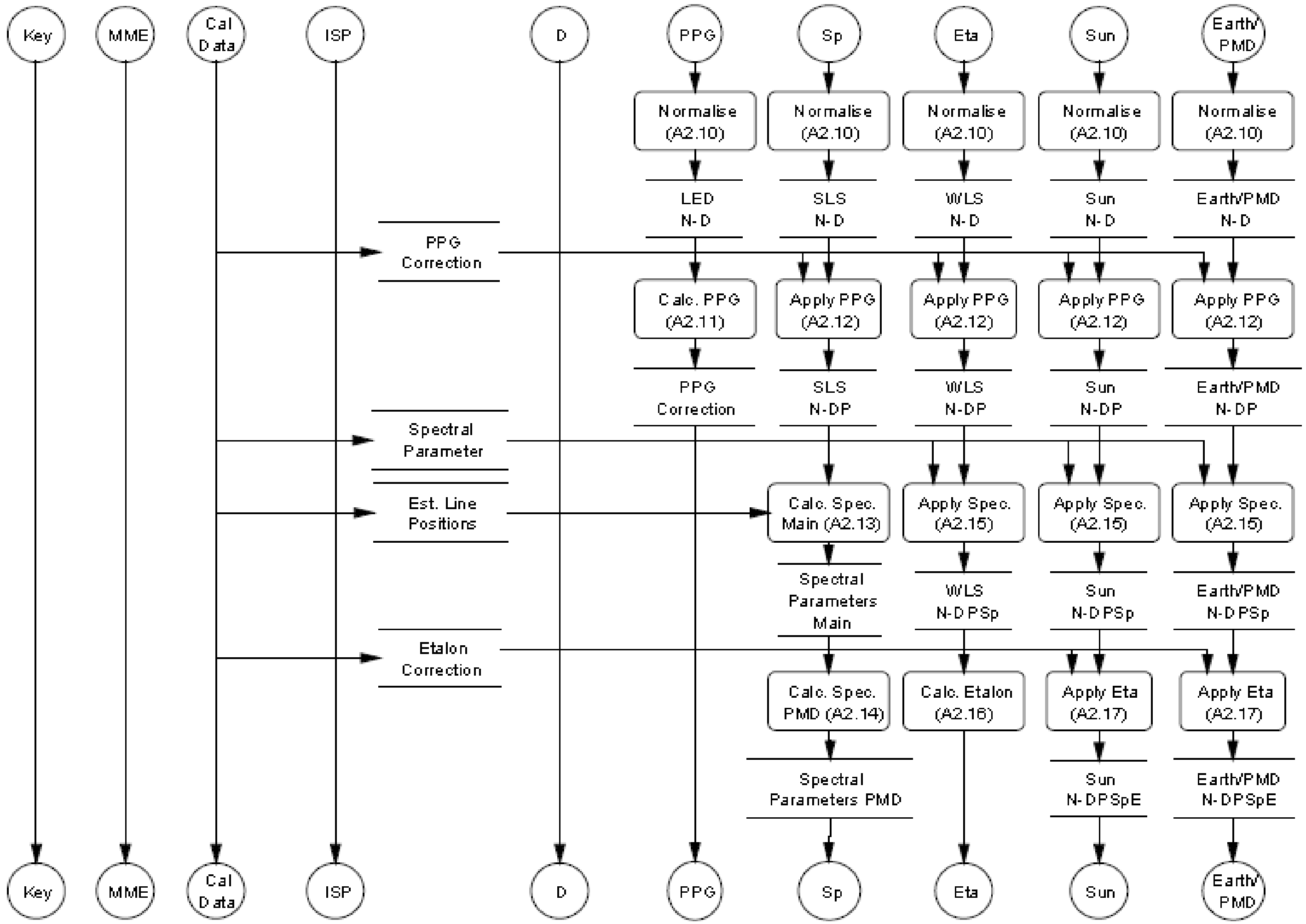

Figure 6: A2 Functional Decomposition: Level 0 to 1a Processor (3).

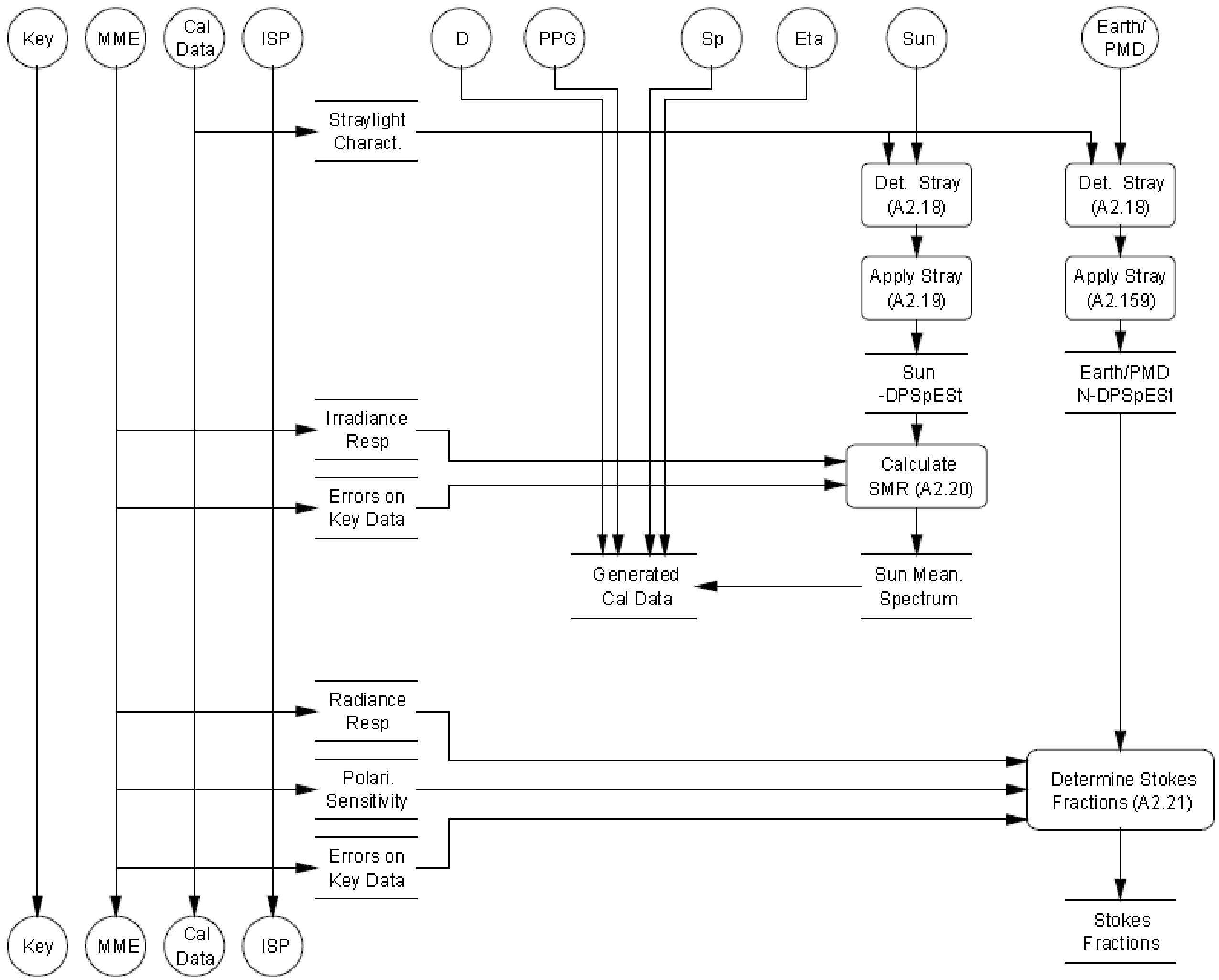

Figure 7: A2 Functional Decomposition: Level 0 to 1a Processor (3).

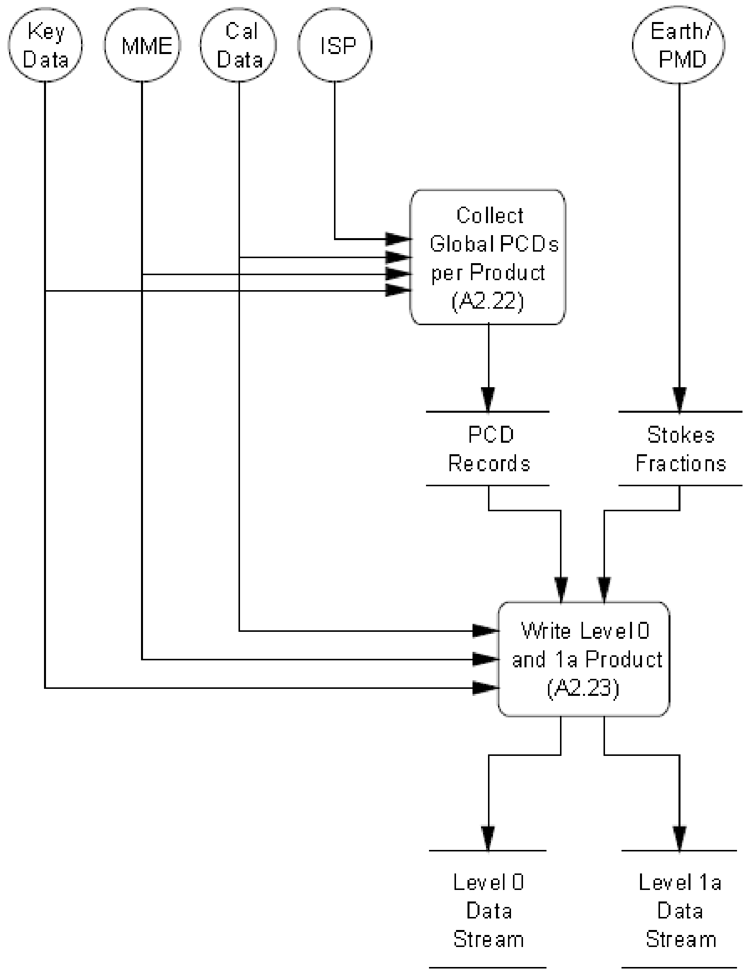

Figure 8: A2 Functional Decomposition: Level 0 to 1a Processor (4).

The solar mean reference spectrum, and atmospheric polarisation state are also determined. Furthermore the geolocation of the measurement is calculated from the appropriate orbit and attitude information, and time correlation information in the level 0 data stream.

Note Any application of calibration parameters in the level 0 to 1a processing should be regarded as interim, to facilitate the generation of new calibration parameters and correction factors. There is no application of calibration parameters to FPA earth observation measurements.

5.2.1.7 Gome-2 Level 0 Data Stream

Level 0 data, the instrument science packets, will be provided to the level 0 to 1a processor as a continuous stream of data packets. In the case of re-processing this data stream is replaced by the level 0 products which have been generated in a previous run of the level 0 to 1a processor. The PGF generates the following output:

Level 1a Data Stream

Depending on the time coverage of the level 0 data stream on input the generated level 1a data stream covers the corresponding time period. The level 0 to 1a processor generates the Level 1a data stream for formatting as specified in [AD4] and [AD5]. These data will be stored in the UMARF and are available for reprocessing purposes.

5.2.2 Read Input Data (A2.0)

Uses Generic Sub-Functions

None

Uses Auxiliary Sub-Functions

None

Data Granule

Initialisation Data
Orbit and Time Correlation Data
Static Auxiliary Data
Key Data
Correction Factor Data
In-flight Calibration Data
Level 0 Data Product or Stream

5.2.2.1 Objective

To read all input data required by the GOME-2 level 0 to 1a processor and to separate the input level 0 data product into scans. Missing data packets and scans are counted and missing data packets flagged.

5.2.2.2 Description

This module reads all initialisation data, orbit and time correlation data, static auxiliary data, key data, correction factors and in-flight calibration data required by the GOME-2 level 0 to 1a processor. In addition the level 0 data product is read and split into individual scans for further processing. The number of missing scans and the number of missing data packets in all valid scans are recorded. A flag is raised for each scan with missing data packets. The beginning and end of each scan and the number of missing scans are determined using the data packet subset counter and the data packet sequence control contained in the Housekeeping data of the Science Data Packet (SDP).

5.2.2.3 Variables

5.2.2.3.1 Read Initialisation Data (A2.0.1)

Preliminary values for the initialisation variables which may be useful for testing purposes are indicated in italics in the References/Remarks column. The initialisation data set used in the generation of a level 1a product is referenced in record GEADR-Initialisation as specified in [AD5].

In addition, a number of MPHR entries (e.g., spacecraft identifier, instrument model, processing centre, processing mode) may also be defined as initialisation variables if required and not in conflict with any higher-level generic requirements. As this is implementation-specific, they are not listed in the table below. The table that follows lists the input from each initialisation data set.

5.2.2.3.1.1 Input from initialisation dataset

Symbol	***Descriptive Name***	***Type***	***Units***	***I/O***	***Source/Destination***	***References/Remarks***
T_{valid}	Temperature selected for valid range key data	d	*K*	i/o	ini/A2.0.4	*278.16*
old_{Dark}	Time after calibration measurement beyond which Dark signal correction parameters are considered old.	i	*days*	i/o	ini/A2.0.6 & various	*1 day (measured once per orbit)*
old_{PPG}	Time after calibration measurement beyond which spectral calibration parameters are considered old.	i	*days*	i/o	ini/A2.0.6 & various	*30 days (measured once per 29-day repeat cycle)*
$\text{old}_{Spectral}$	Time after calibration measurement beyond which spectral calibration parameters are considered old.	i	*days*	i/o	ini/A2.0.6 & various	*2 days (measured once per day)*
old_{Etalon}	Time after calibration measurement beyond which Etalon correction parameters are considered old	i	*days*	i/o	ini/A2.0.6 & various	*2 days (measured once per day)*
old_{SMR}	Time after calibration measurements beyond which the SMR spectrum is considered old.	i	*days*	i/o	ini/A2.0.6 & various	*2 days (measured once per day)*
θ_{term}	Solar zenith angle in the Northern hemisphere which defines the terminator. The solar zenith angle will be decreasing as the satellite approaches the terminator	d	degree	i/o	ini/A2	*108.0*
$\theta_{termDark}$	Solar zenith angle in the Northern hemisphere which defines the terminator with some margin as appropriate for dark signal measurements.	d	degree	i/o	ini/A2.7	*90.0*
$\theta_{termEarth}$	Solar zenith angle in the Northern hemisphere which defines the terminator with some margin as appropriate for Earth measurements.	d	degree	i/o	ini/A2.7	*110.0*
$\theta_{DarkCut}$	Solar zenith angle in the Northern hemisphere which defines the terminator as appropriate for cutting off dark signal measurements.	d	degree	i/o	ini/A2.8	*118.0*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
irrad_flag	Flag to determine which method is to be used for calculation of MMEs for irradiance	enum	–	i/o	ini/A2.1	*1= end-to-end* *2= component 1*
f_{I_R}	Scaling factor for calculation of error on sun-normalised radiance	d	–	i/o	ini/A2.1	*0.8*
$\lambda_{MME,start}$	Start wavelength for Müller Matrix Element wavelength grid	d[B]	nm	i/o	ini/A2.1	*202.0, 298.0, 390.0, 583.0, 290.0, 290.0*
$\lambda_{MME,end}$	End wavelength for Müller Matrix Element wavelength grid	d[B]	nm	i/o	ini/A2.1	*325.0, 421,0, 609.0, 800.0, 810.0, 810.0*
$N_{\psi f}$	Number of viewing angles for which the fine viewing angle grid is specified	w	–	i/o	ini/A2.1	**GIADR-1a-MME** MME_N_PSI_F *21*
N_{ef}	Number of solar elevation angles for which the fine elevation angle grid is specified	w	–	i/o	ini/A2.1	**GIADR-1a-MME** MME_N_E_F *31*
$N_{\varphi f}$	Number of solar azimuth angles for which the fine azimuth angle grid is specified	w		i/o	ini/A2.1	**GIADR-1a-MME** MME_N_PHI_F *33*
ψ_f	Viewing angles which define the fine viewing angle grid	d[$N_{\psi f}$]	degree	i/o	ini/A2.1	***GADR-1a-MME*** MME_PSI_F *–49, –45, …, 0, …, 45, 50*
e_f	Solar elevation angles which define the fine elevation angle grid (Satellite Relative Actual Reference CS)	d[N_{ef}]	degree	i/o	ini/A2.1	**GIADR-1a-MME** MME_E_F *–1.5, –1.4, …, 0, 1.4, 1.5*
φ_f	Solar azimuth angles which define the fine azimuth angle grid (Satellite Relative Actual Reference CS)	d[$N_{\varphi f}$]	degree	i/o	ini/A2.1	**GIADR-1a-MME** MME_PHI_F *317.0, 317.5, …, 332.5, 333.0*
ψ_s	Viewing angle for viewing the internal diffuser plate	d	degree	i/o	ini/A2.1	*+178.616*

Symbol	***Descriptive Name***	***Type***	***Units***	***I/O***	***Source/Destination***	***References/Remarks***
UseZeta	Flag indicating whether to use ζ key data to calculate μ^3. If set to false, μ^3 defaults to 0, which means the U polarisation component will not be considered in the polarisation correction.	bool	–	i/o	ini/A2.1	*0 = do not use ζ* *1 = use ζ* *1*
P_{nm}	Polynomial coefficients for HK conversion to engineering units. HK data are the first 488 words of a data packet, of which *N* are to be converted into engineering units.	d[N,5]	(various)	i/o	ini/A2.2	As specified in [AD6].
ITTable	Integration times corresponding to indices 0…255 in the Science Data Packet.	d[256]	s	i/o	ini/A2.2	See [AD10].
T^{det}_{low}	Lowest nominal detector temperature	d[B]	K	i/o	ini/A2.2	*230.0, 230.0, 230.0, 230.0,230.0, 230.0*
T^{det}_{high}	Highest nominal detector temperature	d[B]	K	i/o	ini/A2.2	*240.0, 240.0, 240.0, 240.0, 240.0, 240.0*
T^{pdp}_{low}	Lowest nominal predisperser temperature	d	K	i/o	ini/A2.2	*268.0*
T^{pdp}_{high}	Highest nominal predisperser prism temperature	d	K	i/o	ini/A2.2	*288.0*
T^{rad}_{low}	Lowest nominal radiator temperature	d	K	i/o	ini/A2.2	*260.0*
T^{rad}_{high}	Highest nominal radiator temperature	d	K	i/o	ini/A2.2	*300.0*
U^{SLS}_{low}	Lowest nominal SLS lamp voltage	d	V	i/o	ini/A2.2	*200.0*
U^{SLS}_{high}	Highest nominal SLS lamp voltage	d	V	i/o	ini/A2.2	*230.0*
I^{SLS}_{low}	Lowest nominal SLS lamp current	d	A	i/o	ini/A2.2	9.5×10^{-3}
I^{SLS}_{high}	Highest nominal SLS lamp current	d	A	i/o	ini/A2.2	10.5×10^{-3}
U^{WLS}_{low}	Lowest nominal WLS lamp voltage	d	V	i/o	ini/A2.2	*7.5*
U^{WLS}_{high}	Highest nominal WLS lamp voltage	d	V	i/o	ini/A2.2	*12.5*

Symbol	***Descriptive Name***	***Type***	***Units***	***I/O***	***Source/Destination***	***References/Remarks***
I^{WLS}_{low}	Lowest nominal WLS lamp current	d	V	i/o	ini/A2.2	*0.355*
I^{WLS}_{high}	Highest nominal WLS lamp current	d	V	i/o	ini/A2.2	*0.425*
$\psi_{SM,0}$	Viewing angle at $n_{SM} = 0$	d	degree	i/o	ini/A2.1, A2.3	As specified in [AD6].
$\psi_{SM,1}$	Viewing angle increment per binary unit in n_{SM}	d	degree/BU	i/o	ini/A2.3	As specified in [AD6].
ψ_{EARTH}	Viewing angle range for earth view	d[2]	degree	i/o	ini/A2.3	*–62.0…+62.0*
ψ_{MOON}	Viewing angle range for moon view	d[2]	degree	i/o	ini/A2.3	*+65.0…+85.0*
ψ_{DARK}	Viewing angle range for dark view	d[2]	degree	i/o	ini/A2.3	*+98.1…+99.1*
ψ_{SLS}	Viewing angle range for SLS view	d[2]	degree	i/o	ini/A2.3	*+166.7…+167.7*
$\psi_{DIFFUSER}$	Viewing angle range for diffuser view	d[2]	degree	i/o	ini/A2.3	*+176.0…+180.0*
ψ_{WLS}	Viewing angle range for WLS view	d[2]	degree	i/o	ini/A2.3	*+187.5…+188.5*
ψ_{Nadir}	Forward scan centre viewing angle range for north polar view	d[2]	degree	i/o	ini/A2.3	*–0.5…+0.5*
ψ_{NorthP}	Forward scan centre viewing angle range for north polar view	d[2]	degree	i/o	ini/A2.3	*43.151…44.151*
ψ_{SouthP}	Forward scan centre viewing angle range for south polar view	d[2]	degree	i/o	ini/A2.3	*–43.628…–42.628*
$\psi_{Scan,min}$	Minimum viewing angle amplitude for a scan to be classified into one of the earth scanning modes	d	A	i/o	ini/A2.2,A2.3	*1.0*
I^{WLS}_{on}	Minimum WLS current for the WLS to be considered “on”	d	A	i/o	ini/A2.2,A2.3	*0.050*
I^{SLS}_{on}	Minimum SLS current for the SLS to be considered “on”	d	A	i/o	ini/A2.2,A2.3	*0.005*
Δt_{SM}	Offset in time of first scan mirror position in packet with respect to UTC timestamp in packet	d	s	i/o	ini/A2.3	*–0.375*
t_{first}	First valid UTC time	d	frac days	i/o	ini/A2.3	*2372.0 30 June 2006*

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
t_{last}	Last valid UTC time	d	fractional days	i/o	ini/A2.3	*10000.0*
C	Number of on-board clock steps per step of SBT_0	i	–	i/o	ini/A2.3	*1 for UTCOption = 2* *256 for UTCOption = 3*
N	Number of different values the SBT counter can assume.	i	–	i/o	ini/A2.3	2^{40}
f_{roll}	Fraction of full SBT counter range to consider for the rollover check	i	–	i/o	ini/A2.3	*16*
UTCOption	Algorithm option to calculate UTC	enum	–	i/o	ini/A2.3	*1*
F_2	Scaling factor for UTC option 2	d	–	i/o	ini/A2.3	256×10^9
F_3	Scaling factor for UTC option 3	d	–	i/o	ini/A2.3	*1.0*
t_{min}	Threshold for minimum mean un calibrated signal per band	w[B]	BU	i/o	ini/A2.4	*1400 (all bands)*
t_{sat}	Saturation threshold per band	d[B]	BU	i/o	ini/A2.4	*52000 (all bands)*
t_{hot}	Hot pixel threshold per band	d[B]	BU	i/o	ini/A2.4	*500 (all bands)*
R_{Sun}	Semi-diameter of the sun	d	m	i/o	ini/A2.1	6.96×10^8 *[AD7]*
R_{Moon}	Semi-diameter of the moon	d	m	i/o	ini/A2.3	1.738×10^6 *[AD7]*
h_0	Height at which satellite and solar elevation and azimuth angles in the topocentric CS are calculated	d	m	i/o	ini/A2.3	*0*
$\Theta_{Sun,Refr}$	Solar zenith angle (Satellite Relative Actual Reference CS) threshold for change of `mp_target` ray tracing model switch	d	degree	i/o	ini/A2.3	*80*
$iray_{Sun-Moon}$	`mp_target` ray tracing model switch for calculation of solar/lunar angles in Satellite Relative Actual Reference CS	i	–	i/o	ini/A2.3	*MP_NO_REF*
$iray_{Earth-LowSZA}$	`mp_target` ray tracing model switch for calculation of topocentric parameters in earth observation mode for solar zenith angles below $\Theta_{Sun,Refr}$	i	–	i/o	ini/A2.3	*MP_NO_REF*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
$iray_{\text{Earth-HighSZA}}$	`mp_target` ray tracing model switch for calculation of topocentric parameters in earth observation mode for solar zenith angles above $\Theta_{\text{Sun,Refr}}$	i	–	i/o	ini/A2.3	MP_NO_REF
freq	`mp_target` frequency of the signal	d	Hz	i/o	ini/A2.3	7.5×10^{14} *(corresponding to 400 nm)*
lon_{SAA}	SAA longitude range (min/max)	d[2]	degree	i/o	ini/A2.7	*–100, 0*
lat_{SAA}	SAA latitude range (min/max)	d[2]	degree	i/o	ini/A2.7	*–50, +10*
$t_{1,\text{sunglint}}$	Threshold for low sunglint risk	d	degree	i/o	ini/A2.7	*15*
$t_{2,\text{sunglint}}$	Threshold for high sunglint risk	d	degree	i/o	ini/A2.7	*5*
ρ_1	Reference angle for rainbow check	d	degree	i/o	ini/A2.7	*140*
ρ_2	Angular limit for rainbow check	d	degree	i/o	ini/A2.7	*3*
t_{stab}^{Dark}	Stabilisation time for dark signal measurements	d	second	i	ini/A2.8	
t_{min}^{Dark}	Minimum duration time for dark signal measurements	d	second	i	ini/A2.8	
$t_{\overline{DS}}$	Threshold for dark signal averaged per band	d[B]	BU/s	i/o	ini/A2.8	*10, 10, 10, 10, 10, 10, 400, 400, 400, 400*
$t_{\overline{\sigma D}}$	Threshold for dark signal read out noise averaged per band	d[B]	BU	i/o	ini/A2.8	*5 (all bands)*
offset	Dark signal electronic offset	i[B]	BU	i/o	ini/A2.8	*1501, 1503, 1495,1492, 1503, 1499*
δ_{dt}	Dark signal detector temperature tolerance	d	K	i/o	ini/A2.9	*0.2*
$t_{\sigma_{dt}}$	Threshold for dark signal detector temperature standard deviation	d	K	i/o	ini/A2.9	*0.2*
$discard_{dt}$	Temperature difference below which a previous dark signal correction is discarded from a data set containing only most recent in-flight calibration data records	i	K	i/o	ini/A2.9	*0.05*

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
SAA_{pix}	Band 1a detector pixel number for SAA correction estimate	i	–	i/o	ini/A2.9	*5*
SAA_{sort}	Number of band 1a detector pixels to be sorted for SAA correction estimate	i	–	i/o	ini/A2.9	*50*
SAA_{thresh}	Threshold signal for SAA detection	d	BU/s	i/o	ini/A2.9	*5*
SAA_1a	Flag indicating whether to apply the additional dark signal correction to band 1a measurements in the SAA	bool	–	i/o	ini/A2.9	*1 = correct* *0 = do not correct*
pe	Number of photo-electrons per BU for each channel	i[B]	BU^{-1}	i/o	ini/A2.9	*960 (all channels)*
PPG_back	Switch for selection of backup source (WLS) in case of LED failure	enum	–	i/o	ini/A2.11	*LED* (See [AD5].)
t_{stab}^{LED}	Stabilisation time for LEDs	d	second	i/o	ini/A2.11	*12*
$t_{\overline{PPG}}$	Threshold for PPG correction averaged per channel	d[B]	–	i/o	ini/A2.11	*0.01*
$t_{\sigma PPG}$	Threshold for standard deviation in PPG per channel	d[B]	–	i/o	ini/A2.11	*0.02*
sm_{LED}	Smoothing width	i	pixel	i/o	ini/A2.11	*5 (must be odd)*
δ_{PPG}	PPG error estimate for each channel	d[B]	–	i/o	ini/A2.12	*0.001*
t_{stab}^{SLS}	Stabilisation time for SLS lamp	d	second	i/o	ini/A2.13	*30*
U_{lvm}^{SLS}	SLS lamp voltage for low voltage mode	d	V	i/o	ini/A2.13	*205*
M	Order of wavelength calibration polynomial per channel. ***Note:*** The number of polynomial coefficients is M + 1.	i[B]	V	i/o	ini/A2.13	*3, 3, 4, 4, 6, 6*
Δ	Search window used for line-finding around first-guess pixel position per channel	$i[B_{FPA},2]$	pix	i/o	ini/A2.13	*channel 1: -9,9* *channel 2: -4,4* *channel 3: -5,5* *channel 4: -8,8* *(pixel offsets with respect to the first guess positions)*

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
S_{req}	Minimum required peak signal for a line to be accepted	i	BU	i/o	ini/A2.13	*80*
w	Width of statistics window around a line per channel	i[BFPA]	pixel	i/o	ini/A2.13	7 (must be odd). Includes one pixel on either side for background subtraction.
$FWHM_{max}$	Maximum full width at half maximum for a line to be accepted per channel	d[BFPA]	pixel	i/o	ini/A2.13	*3.0*
$Skew_{max}$	Maximum skewness for a line to be accepted per channel	d[BFPA	$pixel^3$	i/o	ini/A2.13	*2.0*
$t_{\delta max}$	Threshold for maximum deviation between fitted line positions and true line positions.	d[BFPA]	nm	i/o	ini/A2.13	*0.01, 0.02, 0.05, 0.05*
MapSLS	Flag indicating whether to apply the mapping to external SLS in the main channel spectral calibration	bool	–	i/o	ini/A2.13	*0 = do not perform mapping* *1 = perform mapping*
N_w	Number of spectral windows for cross-correlation algorithm	i	–	i/o	ini/A2.14	*5*
λ_w	Start/end wavelengths for spectral windows	d[2,Nw]	nm	i/o	ini/A2.14	*start:312, 342, 384,446, 555* *end:342, 384,446, 555, 796* *(corresponds to windows approximately 40 pixel wide)*
$\lambda_{E,start}$	Start wavelength for equidistant wavelength grid	d	nm	i/o	ini/A2.14	*300.0*
$\lambda_{E,end}$	End wavelength for equidistant wavelength grid	d	nm	i/o	ini/A2.14	*790.0*
N_E	Number of points in equidistant wavelength grid	i	nm	i/o	ini/A2.14	*65536*
Δ_{max}	Maximum spectral shift allowed for the calibration to be successful	d[BPMD]	pixel	i/o	ini/A2.14	*0.2*
$N_{itermax}^{pmd}$	Maximum number of iterations allowed	d[BPMD]	–	i/o	ini/A2.14	*15*
t_{gof}	Threshold for goodness of fit for PMD spectral calibration	d[BPMD]		i/o	ini/A2.14	*10*

Symbol	***Descriptive Name***	***Type***	***Units***	***I/O***	***Source/Destination***	***References/Remarks***
δ_{pdp}	Pre-disperser prism temperature tolerance	d	K	i/o	ini/A2.15	*0.2*
$t_{\sigma_{pdp}}$	Threshold for pre-disperser prism temperature standard deviation	d	K	i/o	ini/A2.15	*0.2*
$discard_{pdp}$	Temperature difference below which previous spectral calibration parameters are discarded from a data set containing only most recent in-flight calibration data records	d	K	i/o	ini/A2.15	*0.05*
Eta_algo	Etalon correction algorithm selection	enum	–	i/o	ini/A2.16	*Algo1 (see [AD5])*
Eta_back	Switch for selection of backup source (SMR) in case of WLS failure	enum	–	i/o	ini/A2.16	*WLS (see [AD5])*
ETS	Start detector pixel for each channel for use in Etalon correction calculation	i[B]	–	i/o	ini/A2.16	*450, 200, 100, 75, 768, 768*
ETE	End detector pixel for each channel for use in Etalon correction calculation	i[B]	–	i/o	ini/A2.16	*950, 1023, 1023, 1023, 1023, 1023*
t_{stab}^{WLS}	Stabilisation time for WLS lamp	d	s	i/o	ini/A2.16	*60*
f	Fourier frequencies used to deter-mine filter P for each channel.	i[4,B]	–	i/o	ini/A2.16	*0, 3,25, 50 (Values will be fine-tuned per channel!)*
smLEDtype	Switch for selection of smoothing function	enum	–	i	A2.0.1	*0 = triangular* *1 = polynomial*
sm_{LED}	Smoothing width	i	pixels	i/o	ini/A2.16	*5*
$t_{\overline{RES}}$	Threshold for mean residual etalon per channel	d[B]	–	i/o	ini/A2.16	*0.01*
$t_{\sigma_{RES}}$	Threshold for standard deviation of residual etalon per channel	d[B]	–	i/o	ini/A2.16	*0.02*
$t_{\overline{rpps}}$	Threshold for residual pixel level structure per channel	d[B]	–	i/o	ini/A2.16	*0.01*
$t_{\sigma_{rpps}}$	Threshold for standard deviation of residual pixel level structure per channel	d[B]	–	i/o	ini/A2.16	*0.02*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
δ_{Eta}	Etalon error estimate for each channel	d[B]	-	i/o	ini/A2.17	*0.01*
δ_{Stray}	Stray light error estimate for each channel	d[B]	–	i/o	ini/A2.19	*0.01*
δI	Intensity threshold for difference in intensity pairs	d	–	i/o	ini/A2.20	*0.1*
e_{central}	Central elevation angle of the Sun observation mode detector readouts	d	degree	i/o	ini/A2.20	*0.0*
δe	Maximum deviation of solar elevation from central angle	d	degree	i/o	ini/A2.20	*1.5*
t_{Nsun}	Threshold for number of detector readouts in Sun observation mode which pass the intensity check test.	i	–	i/o	ini/A2.20	*15*
c	Speed of light.	d	m/s	i/o	ini/A2.20	2.99792458×10^8
N_{PMD}	Total number of PMD bands	w	–	i/o	ini/AG.18 A2.21	*15*
$S_{s,req}$	Minimum required PMD-s signal	d	BU	i/o	ini/A2.21	*50*
$S_{p,req}$	Minimum required PMD-p signal	d	BU	i/o	ini/A2.21	*60*
M_{SSP}	Number of zenith angle/wave-length pairs for single-scattering parameterisation	i	–	i	ini/A2.21	*6*
$\theta_{Sun,SSP}$	Solar zenith angle for single-scattering parameterisation	d[M_{SSP}]	degree	i	ini/A2.21	*0.0, 18.0, 36.9,53.1, 66.4, 75.5*
λ_{SSP}	Wavelength of single-scattering value corresponding to $\theta_{\mathrm{Sun,SSP}}$	d[M_{SSP}]	nm	i	ini/A2.21	*297.8, 298.0, 298.7, 299.5, 301.5, 303.5*
$P_{\mathrm{SS,min,BadStokes}}$	Minimum single-scattering degree of polarisation for Stokes fractions to be checked	d	–	i	ini/A2.21	*0.1*
$\lambda_{\mathrm{min,BadStokes}}$	Minimum PMD band wavelength for Stokes fractions to be checked	d	nm	i	ini/A2.21	*600*
δ_q	Tolerance for Stokes fraction check	d	–	i	ini/A2.21	*0.01*

Symbol	***Descriptive Name***	***Type***	***Units***	***I/O***	***Source/Destination***	***References/Remarks***
Δ_{depol}	Depolarisation parameter for Rayleigh scattering	d	–	i	ini/A2.21	0.0657, valid at 290 nm [GD6]
i_{Scene}	Index of PMD band from which scene variability is derived (zero-based)	i	–	i	ini/A2.21	*8*
$q_{SS,min}$	Lower threshold for single-scattering Stokes fraction q_{SS} to avoid singularity in $u_{SS}/q_{SS.}$	d	–	i/o	ini/A2.21	*0.05*
$\cos(2\chi)_{SS,\ min}$	Minimum cosine of two times the polarisation angle for Rayleigh scattering below which q = 0	d[R_{FPA}]	–	i/o	ini/A2.21	*0.026*
m_{qc}	PMD signal ratio tolerance for accepting correction signals for special geometry readouts	d	–	i/o	ini/A2.21	*0.1*
N^{qc}	Minimum number of PMD correction signal ratios accumulated until writing of mean values to COR file for all high resolution viewing angles ψ^h and MME wavelength grid *i*	d	–	i/o	ini/A2.21	*3*
$\Delta^{t,qc}$	Maximum number of days for accumulation of PMD signal response correction values	d	–	i/o	ini/A2.21	*2*
$\Delta^{h,qc}$	Maximum difference between actual viewing angle for PMD readout *j* and nearest neighbour grid point *h* on high resolution viewing angle grid	d	–	i/o	ini/A2.21	*0.1*

5.2.2.3.2 Read Orbit and Time Correlation Data (A2.02)

The orbit data set used in the generation of a level 1a product is referenced in record **GEADR-1a-Orbit** as specified in [AD5].

5.2.2.3.2.1 Input from orbit dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
orbitno	Orbit number	i	-	i/o	orb/A2.23.3	**MPHR** ORBIT_START ORBIT_END
t_0	UTC of initial osculating state vector (processing format): |fractional days after 1 Jan 2000 ⊗UT1 = UT1–UTC	d[2]	[day] [s]	i/o	orb/AG.1	*mjdp* assumed to be zero
x_0	Initial Cartesian osculating position vector (earth-fixed CS)	d[3]	m	i/o	orb/AG.1	*pos*
v_0	Initial Cartesian osculating velocity vector (earth-fixed CS)	d[3]	m/s	i/o	orb/AG.1	*vel*

The time correlation data set, used if option 3 for the calculation of the UTC time grid is selected, is referenced in record **GEADR-1a-TimeCorrelation** as specified in [AD5].

5.2.2.3.2.2 Input from time correlation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
UTC_0	UTC for time correlation	d	fractional days	i/o	orb/A2.3.2	Only for A2.3.2 UTC option 3
SBT_0	SBT for time correlation	d	2^{-16} seconds	i/o	orb/A2.3.2	Only for A2.3.2 UTC option 3
T_s	Time increment for time correlation	d	-	i/o	orb/A2.3.2	Only for A2.3.2 UTC option 3

5.2.2.3.3 Read Static Auxiliary Data (A2.03)

The static auxiliary data sets used in the generation of a level 1a product are referenced in records **GEADR-Static** as specified in [AD5].

5.2.2.3.3.1 Input from static auxiliary dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
NE_{lat}	Number of latitudes in elevation dataset	i	-	i/o	stat/A2.6.3	
NE_{lon}	Number of longitudes in elevation dataset	i	-	i/o	stat/A2.6.3	
E_{lat}	Latitude grid for *Elev*	d[NE_{lat}]	degree	i/o	stat/A2.6.3	
E_{lon}	Longitude grid for *Elev*	d[NE_{lon}]	degree	i/o	stat/A2.6.3	
Elev	Elevation	d[NE_{lat}, NE_{lon}]	m	i/o	stat/A2.6.3	

The static auxiliary data sets used in the generation of a level 1a product are referenced in records **GEADR-Static** as specified in [AD5].

5.2.2.3.3.2 Input from static auxiliary dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
NM_{lat}	Number of latitudes in Land Sea Mask	i		i/o	stat/AG.8	
NM_{lon}	Number of longitudes in Land Sea Mask	i		i/o	stat/AG.8	
Mlat	Latitude grid for *LSM*	d[NM_{lat}]	degrees	i/o	stat/AG.8	
M_{lon}	Longitude grid for *LSM*	d[NM_{lon}]	degrees	i/o	stat/AG.8	
LSM	Land Sea Mask	d[NM_{lat}, NM_{lon}]		i/o	stat/AG.8	

5.2.2.3.4 Read Key Data (A2.0.4)

The Key Data set used in the generation of a level 1a product is referenced in record GEADR-KeyData as specified in [AD5]. Key data file names are indicated in the last column in italics. The last part of the key data file name is omitted: this distinguishes between main channels and PMD channels and specifies the instrument model.

5.2.2.3.4.1 Input from key dataset describing angular dependencies

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
N_ψ	Number of viewing angles for which calibration key data are measured.	w	–	i/o	key/A2.1	*POL_CHI, POL_KAPPA*
N_e	Number of solar elevation angles selected from calibration key data	w	–	i/o	key/A2.1	*BSDF_AIRR Key data may contain more angles.* N_e *is the number of selected angles (see text).*
N_φ	Number of solar azimuth angles selected from calibration key data	w	–	i/o	key/A2.1	*BSDF_AIRR Key data may contain more angles.* N_φ *is the number of selected angles (see text).*
ψ	Viewing angles for which calibration key data are measured	d[Nψ]	degree	i/o	key/A2.1	*POL_CHI, POL_KAPPA*
e	Solar elevation angles for which calibration key data are measured	d[Ne]	degree	i/o	key/A2.1	*BSDF_AIRR*
φ	Solar azimuth angles for which calibration key data are measured	d[Nϕ]	degree	i/o	key/A2.1	*BSDF_AIRR*

5.2.2.3.4.2 Input key dataset describing polarisation sensitivity

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
η^n	Intensity ratio, s-polarised to p-polarised light, for exact nadir direction	d[D,B]	–	i/o	key/A2.1	*POL_ETA*
ζ^n	Intensity ratio, –45° to +45° polarised light, for exact nadir direction	d[D,B]	–	i/o	key/A2.1	*POL_ZETA* *Only used if UseZeta = 1*
α^n	Sensitivity ratio of PMD-s to PMD-p for s-polarised and p- polarised light respectively, for exact nadir direction	d[D,B]	–	i/o	key/A2.1	*POL_ALPHA*
β^n	Normalised sensitivity of PMD-p to s-polarised light, for exact nadir direction	d[D,B]	–	i/o	key/A2.1	*POL_BETA*
γ	Normalised sensitivity of PMD-s top-polarised light. ***Note:*** This normalisation is with respect to the sensitivity of PMD-p to p-polarised light, the scan angle dependence in this quantity cancels from the equation.	d[D]	–	i/o	key/A2.1	*POL_GAMMA*
χ	Viewing angle dependence of η, α and β with respect to nadir	d[D,B,Nψ]	–	i/o	key/A2.1	*POL_CHI*
χ	Viewing angle dependence of ζ with respect to nadir	d[D,B,Nψ]	–	i/o	key/A2.1	*POL_CHI_ZETA*
ε_η^n	Relative error in intensity ratio, s-polarised to p-polarised light, for exact nadir direction	d[D,B]	–	i/o	key/A2.1	*POL_ETA*
ε_χ	Relative error in viewing angle dependence of η, α and β with respect to nadir	d[D,B]	–	i/o	key/A2.1	*POL_CHI*

5.2.2.3.4.3 *Input from key dataset describing radiance sensitivity*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
R_{u}^{00}	Radiance response function for unpolarised light and exact nadir direction	d[D,B]	$BU.s^{-1}/(W.srcm^{3})$	i/o	key/A2.1	*RA_ABS_RAD*
κ	Viewing angle dependence of radiance response function	d[D,B, Nψ]	–	i/o	key/A2.1	*POL_KAPPA*
$\varepsilon\_R_{u}^{00}$	Relative error in radiance response function for unpolarised light and exact nadir direction	d[D,B]	–	i/o	key/A2.1	*RA_ABS_RAD*
ε_κ	Relative error in viewing angle dependence of radiance response function	d[D,B]	–	i/o	key/A2.1	*POL_KAPPA*

5.2.2.3.4.4 *Input from key dataset describing irradiance sensitivity*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
I_{u}^{0}	Irradiance response function for zero elevation and azimuth angles	d[D,B]	$BU.s^{-1}/(W.srcm^{3})$	i/o	key/A2.1	*RA_ABS_IRR*
C	Correction factor for azimuth and elevation angle dependence of irradiance response	d[D,B, N_e,N_φ]	–	i/o	key/A2.1	*BSDF_AIRR After constructing a regular azimuth/elevation grid as described below*.
BSDF_s	BSDF of calibration unit in response to s-polarised light	d[D,B]	–	i/o	key/A2.1	*BSDF_CU_S*
BSDF_p	BSDF of calibration unit in response to p-polarised light	d[D,B]	–	i/o	key/A2.1	*BSDF_CU_P*
$\varepsilon\_I_{u}^{0}$	Relative error in irradiance response function for zero elevation and azimuth angles	d[D,B]	–	i/o	key/A2.1	*RA_ABS_IRR*
ε_C	Relative error in correction factor for azimuth and elevation angle dependence of irradiance response	d[D,B]	–	i/o	key/A2.1	*BSDF_AIRR*
ε_*BSDF*	Relative error in BSDF of calibration unit	d[D,B]	–	i/o	key/A2.1	*BSDF_CU_S* *BSDF_CU_P*

5.2.2.3.4.5 Key data for wavelength calibration

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
A_{Ref}	Reference polynomial coefficients for spectral calibration as read from key data	d[B,max(M)]	nm	i	key	*WL_MAIN* *WL_PMD_P_MON* *WL_PMD_S_MON*
λ^{REF}_{PMD}	PMD channel wavelength grid	$d[D_{PMD},B_{PMD}]$	nm	i	key/A2.14	*WL_PMD_P_MON* *WL_PMD_S_MON*
Ktot	Number of used SLS lines	i	-	i/o	key/A2.13	*WL_LINEPOS_MAIN*
λ	Position of SLS line given as vacuum wavelength	$d[K_{tot}]$	nm	i/o	key/A2.13	*WL_LINEPOS_MAIN* this is channel independent
i_0	Position of SLS lines given as fractional pixel number per main channel (for the instrument in vacuum)	$d[K_{cha}, B_{FPA}]$	pixel	i/o	key/A2.13	*WL_LINEPOS_MAIN* to be used as first guess position for line finding
N_q	Number of stokes fractions for SLS radiance at the output of the GOME-2 Calibration Unit	i	-	i/o	key/A2.14	*POL_STOKES_SLS*
λ_{qc}	Wavelength grid associated with the Stokes fractions for SLS output of the GOME-2 Calibration Unit	d[Nq]	nm	i/o	key/A2.14	*POL_STOKES_SLS*
q_c	Stokes fractions for SLS radiance at the output of the GOME-2 Calibration Unit	d[Nq]	-	i/o	key/A2.14	*POL_STOKES_SLS*
N_{pix}	Maximum number of detector pixels for which PMD slit function is defined (for a given wavelength)	i	-	i/o	key/A2.14	*WL_SLIT_PMD_P* *WL_SLIT_PMD_S*
N_{wl}	Number of wavelengths for which the PMD slit function is given	i	-	i/o	key/A2.14	*WL_SLIT_PMD_P* *WL_SLIT_PMD_S*
λ_F	Wavelength for PMD slit function	$d[N\mathrm{wl}]$	nm	i/o	key/A2.14	*WL_SLIT_PMD_P* *WL_SLIT_PMD_S*
F	PMD slit function	$d[N_{pix}, N_{wl}]$	-	i/o	key/A2.14	*WL_SLIT_PMD_P* *WL_SLIT_PMD_S*
λ_{OL}	Wavelength of main channel separation (50% / 50% intensity point)	d[3]	nm	i/o	key/A2.14	*WL_OVERLAP* the elements will be referenced as λ_{OL1-2}, λ_{OL2-3}, and λ_{OL3-4} below.

5.2.2.3.4.6 Key data for etalon correction

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
WLS_{ref}	Reference WLS spectra, corrected for PPG	d[D,B]	BU/s	i/o	key/A2.16	*RA_WLS*
λ_{ref}	Wavelength grid associated with the reference WLS measurements	d[D	nm	i/o	key/A2.16	*RA_WLS*
SMR_{ref}	Reference SMR spectra, corrected for PPG	d[D	photons/(s.cm^2.nm)	i/o	key/A2.16	*SMR_REF (Note: this data is derived after launch)*
λ_{SMRref}	Wavelength grid associated with the reference WLS measurements	d[D	nm	i/o	key/A2.16	*SMR_REF (Note: this data is derived after launch)*

5.2.2.3.4.7 Key data for stray light calculation

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
F	Uniform stray light fraction per channel (intra-channel only)	d[B]	–	i/o	key/AG.16	*SS_UNIF*
N^G	Number of stray light ghosts for each channel	i[B]	–	i/o	key/AG.16	*SS_INTRA*
I	Polynomial coefficients describing the intensity of stray light ghosts	d[3,N^G,B]	–	i/o	key/AG.16	*SS_INTRA*
p	Polynomial coefficients describing the location of stray light ghosts	d[3,N^G,B]	–	i/o	key/AG.16	*SS_INTRA*

5.2.2.3.4.8 *Key data for field of view*

Symbol	**Descriptive Name**	**Type**	**Units**	**I/O**	**Source/Destination**	**References/Remarks**
IFOVψ	Across-track (dispersion direction) instantaneous field of view	d	degree	i/o	key/AG.2.2	*FOV_SIZE*
IFOVy	Along-track (cross-dispersion direction) instantaneous field of view	d	degree	i/o	key/AG.2.2	*FOV_SIZE*

5.2.2.3.4.9 *Key data for valid wavelength range*

Symbol	**Descriptive Name**	**Type**	**Units**	**I/O**	**Source/Destination**	**References/Remarks**
$\lambda_{valid,start}$	Start wavelength of valid data per channel	d[B]	nm	i/o	key/A2.23.3	*VALID_RANGE* ***GIADR-Channels*** START_VALID_WAVELENGTHS ***Note***: Select values for temperature T_{valid}
$\lambda_{valid,end}$	End wavelength of valid data per channel	d[B]	nm	i/o	key/A2.23.3	*VALID_RANGE* ***GIADR-Channels*** START_VALID_WAVELENGTHS ***Note***: Select values for temperature T_{valid}
$i_{valid,start}$	Start pixel of valid data per channel	d[B]	nm	i/o	key/A2.23.3	*VALID_RANGE* ***GIADR-Channels*** START_VALID_WAVELENGTHS ***Note***: Select values for temperature T_{valid}
$i_{valid,end}$	End pixel of valid data per channel	d[B]	nm	i/o	key/A2.23.3	*VALID_RANGE* ***GIADR-Channels*** START_VALID_WAVELENGTHS **Note**: Select values for temperature T_{valid}

5.2.2.3.5 Read Correction Factor Data (A2.0.5)

The correction factor data set used in the generation of a level 1a product is referenced in record GEADR-1a-CorrectionFactor of the product as specified in [AD5].

5.2.2.3.5.1 Input from correction factor dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
m	M-factor appropriate to the light path of the earth shine measurements.	d[D,B]	–	i/o	corr/A2.1	*default value 1.0 at the beginning of the in-orbit life of GOME-2*
m_cu	M-factor appropriate to the light path of the solar measurements including the calibration unit.	d[D,B]	–	i/o	corr/A2.1	*default value 1.0 at the beginning of the in-orbit life of GOME-2*
λ^{mfac}	Wavelength grid on which m-factors are supplied.	d[D,B]	nm	i/o	corr/A2.1	
ψ^h	High resolution viewing-angle grid	d[N_{PMD},$N_{\psi h}$]	–	i/o	corr/A2.1	
$\overline{M^{D}_{i\Psi^h}}$	Default correction from PMD signal ratio from special geometries per high resolution viewing angle *h* and MME wavelength grid *i*	d[N_{PMD},$N_{\psi h}$]	–	i/o	corr/A2.1	
$M^{D}_{i\Psi^h}$	Correction from PMD signal ratio from special geometries per high resolution viewing angle *h* and MME wavelength grid *i*	d[N_{PMD},$N_{\psi h}$]	–	i/o	corr/A2.1	

5.2.2.3.6 Read In-Flight Calibration Data (A2.0.6)

The in-flight calibration data set used in the generation of a level 1a product is referenced in record VEADR-In Flight Cal of the product, see [AD5].

5.2.2.3.6.1 Input from In-flight calibration dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
DS_{start}	Start UTC date/time of valid Dark calibration mode measurements	d	fractional days	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark START_UTC_DARK

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
DS_{end}	End UTC date/time of valid Dark calibration mode measurements	d	fractional days	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark END_UTC_DARK
DS_{IT}	Integration time for which dark signal correction is valid	d[B]	s	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark INTEGRATION_TIME
DS_{dt}	Mean detector temperature for which dark signal correction is valid	d[B]	K	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark FPA_TEMP
$DS_{transfer}$	*pmd_transfer* mode for which dark signal correction is valid	d	–	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark PMD_TRANSFER
$DS_{readout}$	*pmd_readout* mode for which dark signal correction is valid	d	–	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark PMD_READOUT
DS	Dark signal correction	d[D,B]	BU	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark DARK_SIGNAL
σ_D	Standard deviation in dark signal readout values equivalent to readout noise	d[D,B]	BU	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark DARK_READOUT_NOISE
$\overline{DS}$	Dark signal correction averaged per band.	d[B]	BU	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-**Dark PCD_DARK AV_DARK
$\overline{\sigma_D}$	Dark signal correction readout noise averaged per band.	d[B]	BU	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-Dark** PCD_DARKAV_DARK_NOISE
$F_{\overline{DS}}$	Flag indicating whether dark signal correction averaged per band exceeds specified threshold	bool[B]	–	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-Dark** PCD_DARK F_AV_DARK 1 = exceeds 0 = does not
$F_{\overline{\sigma_D}}$	Flag indicating whether dark signal correction readout noise averaged per band exceeds specified threshold	bool[B]	–	i/o	ifc/A2.9 A2.23.2	**VIADR-1a-Dark** PCD_DARK F_AV_DARK 1 = exceeds 0 = does not

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
F_E^{miss}	Flag indicating that missing mean Dark calibration mode measurements have been filled by interpolation or that one complete band is missing	enum[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Dark** PCD_DARK F_DARK_MISS
LED_{start}	Start UTC date/time of valid LED (or WLS if PPG_back = WLS) calibration mode measurements	d	fractional days	i/o	ifc/A2.9, A2.23.2	**VIADR-1a-PPG** START_UTC_PPG
LED_{end}	End UTC date/time of valid LED (or WLS if PPG_back=WLS) calibration mode measurements	d	fractional days	i/o	ifc/A2.9, A2.23.2	**VIADR-1a-PPG** END_UTC_PPG
PPG	Pixel to Pixel Gain correction	d[D,B]	–	i/o	ifc/A2.9, A2.23.2	**VIADR-1a-PPG** PPG
PPG_back	Switch for selection of backup source (WLS) in event of LED failure	enum	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPGPPG_BACK
$\overline{PPG}$	Mean PPG correction per channel DOPE	d[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPGAV_PPG
σ_{PPG}	Standard deviation of PPG per channel	d[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPGSTDDEV_PPG
$F_{\overline{PPG}}$	Flag indicating whether PPG averaged per channel exceeds specified threshold	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPG F_AV_PPG 1 = exceeds 0 = does not
F σ_{PPG}	Flag indicating whether PPG averaged per channel exceeds specified threshold	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPGF_AV_PPG 1 = exceeds 0 = does not
FσPPG	Flag indicating whether standard deviation of PPG per channel exceeds specified threshold	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPGF_STDDEV_PPG 1 = exceeds 0 = does not

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
F_{PPG}^{miss}	Flag indicating that missing mean LED calibration mode measurements have been filled by interpolation or that one complete channel is missing	enum[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPG F_PPG_MISS
F_{PPG}^{LED}	LED status flag	b	–	i/o	ifc/A2.23.2	**VIADR-1a-PPG** PCD_PPGF_PPG_LED See [AD9]
SLS_{start}	Start UTC date/time of valid SLS calibration mode measurements	d	fractional days	i/o	ifc/A2.15 A2.23.2	**VIADR-1a-Spec** START_UTC_SLS
SLS_{end}	End UTC date/time of valid SLS calibration mode measurements	d	fractional days	i/o	ifc/A2.15 A2.23.2	**VIADR-1a-Spec** END_UTC_SLS
SLS*pdp*	Mean pre-disperser prism temperature for which spectral calibration is valid	d	K	i/o	ifc/A2.15 A2.23.2	**VIADR-1a-Spec** PDP_TEMP
a	Polynomial coefficients for spectral calibration	d[B,max(M)]	nm	i/o	ifc/A2.15 A2.23.2	**VIADR-1a-Spec** POLY_COEFF_FPA POLY_COEFF_PMD see equation (75)
N_{lines}	Number of lines accepted for use in spectral calibration per channel.	w[B_{FPA}]	–	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECN_LINES
δ_{max}	Maximum deviation between fitted and true line position per channel	d[B_{FPA}]	nm	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECMAX_LINE_DEV
$\bar{\delta}$	Average deviation between fitted and true line position per channel	d[B_{FPA}]	nm	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECAV_LINE_DEV
δ	Deviation between fitted line position and true line positions.	d[N_{lines}, B_{FPA}]	nm	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECLINE_DEV

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
F_{lines}	Flag indicating whether number of lamp lines accepted for use in spectral calibration is below order of wavelength calibration polynomial lM per channel.	bool [B_{FPA}]	–	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECF_N_LINES 1 = number of lines too low 0 = number of lines sufficient
$F_{\delta max}$	Flag indicating whether maximum deviation between fitted line positions and true line positions exceeds specified threshold.	bool [B_{FPA}]	–	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECF_MAX_LINE_DEV 1 = exceeds 0 = does not
F^{miss}_{SLS}	Flag indicating that no spectral calibration was generated due to missing mean SLS mode measurements per channel	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECF_SPEC_MISS 1 = no spectral calibration for given channel 0 = not missing
N_{iter}	Number of iterations required for PMD spectral calibration per channel.	w[BPMD]	–	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECN_ITERATION
F_{noconv}	Flag indicating that PMD spectral calibration has not converged, per channel	bool [BPMD]	–	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECF_NO_CONVERGENCE 1 = not converged 0 = converged
F_{gof}	Flag indicating whether goodness of fit for PMD spectral calibration is above specified threshold (fit too bad)	bool [BPMD]	–	i/o	ifc/A2.23.2	**VIADR-1a-Spec** PCD_SPECF_GOF 1 = goodness of fit too high 0 = goodness of fit acceptable
WLS_{start}	Start UTC date/time of valid WLS (or Sun if Eta_back = Sun) calibration mode measurements	d	fractional days	i/o	ifc/A2.17 A2.23.2	**VIADR-1a-Etalon** START_UTC_WLS
WLS_{end}	End UTC date/time of valid *WLS* (or *Sun* if *Eta_Back* = *Sun*) calibration mode measurements	d	fractional days	i/o	ifc/A2.17 A2.23.2	**VIADR-1a-Etalon** START_UTC_ WLS

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
λ^{ETN}	Wavelength grid for the measurements from *WLS* calibration mode and the Etalon correction	d[D,B]	nm	i/o	ifc/A2.17 A2.23.2	**VIADR-1a-Etalon** LAMBDA_ ETALON
ETN	Etalon correction	d[D,B]	BU/s	i/o	ifc/A2.17 A2.23.2	**VIADR-1a-Etalon** ETALON
Eta_algo	Etalon correction algorithm selection	enum	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON ETALON_BACK
Eta_back	Switch for selection of backup source (SMR) in case of WLS failure	enum	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON E TALON_ALGO
RES	Mean residual etalon per channel	d[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON AV_ETALON
σ_{RES}	Standard deviation of residual etalon per channel	d[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON STDDEV_ETALON
cppg	Mean residual structure at a pixel level	d[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON AV_RESIDUAL
σ_{cppg}	Standard deviation of residual structure at a pixel level	d[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON STDDEV_RESIDUAL
F_{RES}	Flag indicating whether mean residual etalon exceeds specified threshold per channel	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALONF_AV_ETALON 1 = exceeds 0 = does not
$F_{\sigma RES}$	Flag indicating whether standard deviation of residual etalon exceeds specified threshold per channel	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON F_STDDEV_ ETALON 1 = exceeds 0 = does not

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
$F_{\overline{cppg}}$	Flag indicating whether mean residual pixel level structure exceeds specified threshold per channel	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALONF_AV_RESIDUAL 1 = exceeds 0 = does not
$F_{\sigma cppg}$	Flag indicating whether standard deviation in residual pixel level structure exceeds specified threshold per channel	bool[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON F_STDDEV_RESIDUAL 1 = exceeds 0 = does not
F^{miss}_{ETA}	Flag indicating that missing mean WLS calibration mode measurements have been filled by interpolation or that one complete channel is missing	enum[B]	–	i/o	ifc/A2.23.2	**VIADR-1a-Etalon** PCD_ETALON F_ETALON_MISS
Sun_{start}	Start UTC date/time of valid Sun calibration mode measurements	d	fractional days	i/o	ifc/A2.23.2	**VIADR-SMR** START_UTC_SUN
Sun_{end}	End UTC date/time of valid Sun calibration mode measurements	d	fractional days	i/o	ifc/A2.23.2	**VIADR-SMR** END_UTC_SUN
Sun_{trans}	PMD transfer mode associated with SMR	enum	–	i/o	ifc/A2.23.2	**VIADR-SMR** PMD_TRANSFER
Sun_{read}	PMD readout mode associated with SMR	enum	–	i/o	ifc/A2.23.2	**VIADR-SMR** PMD_READOUT
λ^{SMR}	SMR wavelength grid after Doppler correction	d[D,B]	–	i/o	ifc/A2.23.2	**VIADR-SMR** LAMBDA_SMR
SMR	Solar Mean Reference spectrum	d[D,B]	photons/(s.cm^2.nm)	i/o	ifc/A2.23.2	**VIADR-SMR** SMR
E_{SMR}	Absolute error on the Solar Mean Reference spectrum	d[D,B]	photons/(s.cm^2.nm)	i/o	ifc/A2.23.2	**VIADR-SMR** E_SMR

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
$\varepsilon^{BU/s}_{Sun}$	Relative error in the mean of the *Nsun* solar measurements having passed the intensity and consistency checks, before correction for the irradiance response of the instrument	d[D,B]	–	i/o	ifc/A2.23.2	**VIADR-SMR** E_REL_SUN
N_{sun}	Number of detector readouts in Sun observation mode which pass the intensity check test.	w	–	i/o	ifc/A2.23.2	**VIADR-SMR** PCD_SMR N_INTENSITY
F_{Nsun}	Flag indicating that number of detector readouts in Sun observation mode passing the intensity check test is too low.	bool	–	i/o	ifc/A2.23.2	**VIADR-SMR** PCD_SMR F_N_INTENSITY 1 = number of spectra too low 0 = number of spectra sufficient
F^{miss}_{Sun}	Flag indicating that no SMR was generated due to missing mean Sun mode measurements per channel	bool[B]	–	i/o	ifc	**VIADR-SMR** PCD_SMR F_SMR_MISS 1 = no SMR for given channel 0 = no missing

5.2.2.3.7 Read Level 0 Input Data, Separate Scans and Generate PCDs (A2.0.7)

5.2.2.3.7.1 Local Variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
k	Scan index counter	i	–	t	–	

5.2.2.3.7.2 Input from Level 0 Data Stream

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
HK	Housekeeping data	w[488]	–	i/o	lv0/A2.2 and various	**MDR-1a-*ISP_HEAD** ***Note***: See [AD9] for the location of specific quantities within HK and Spectral data. 16 data packets per scan, HK data are the first 488 words of a data packet.
S	Spectral data	w[8880]	–	i/o	lv0/various	**MDR-1a- BAND_*** Comprises all remaining spectral data in the data packet. ***Note***: See [AD9] for the location of specific quantities within HK and Spectral data. 16 data packets per scan, HK data are the first 488 words of a data packet.
seq	Data packet sequence control	i	–	i	lv0	*HK, range 0...16383*
sub	Data packet subset counter	i	–	i	lv0	*HK, range 0…15*

5.2.2.3.7.3 Global PCDs per Product

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
N_{scan}	Number of scans in the product	w	–	g	A2.22	
N_{miss_dp}	Number of missing data packets invalid scans	w	–	g	A2.22	
N_{val_dp}	Number of valid scans with missing data packets	w	–	g	A2.22	
N_{miss_scan}	Number of missing scans	w	–	g	A2.22	

5.2.2.3.7.4 Output per Scan

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
F_{miss_dp}	Flag indicating missing data packets in scan	bool	–		A2.23.1	MDR*PCD_BASICF_MISS 0 = none missing 1 = missing

5.2.2.3.7.5 Output per Product

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
i_{start}	Start pixel of the band in a specified channel	w[B]	–	o	A2.23.3	**GIADR-1a-Bands** START_PIXEL
i_{number}	Number of pixels in the specified band	w[B]	–	o	A2.23.3	**GIADR-1a-Bands** NUMBER_OF_PIXELS

5.2.2.4 Algorithm

READ INITIALISATION DATA (A2.0.1)

The Initialisation Data listed in Section 5.2.2.3 are read from the Initialisation Data storage location and made available for use in Level 0 to 1a Processing (A2).

READ ORBIT AND TIME CORRELATION DATA (A2.0.2)

The Orbit and, if Option 3 of Determine UTC Time Grid (A2.3.2) is selected, the Time Correlation Data listed in Section 5.2.2.3 are read from the Orbit and Time Correlation Data storage location and made available for use in Level 0 to 1a Processing (A2).

READ STATIC AUXILIARY DATA (A2.0.3)

The Static Auxiliary Data listed in Section 5.2.2.3 are read from the Static Auxiliary Data storage location and made available for use in Level 0 to 1a Processing (A2).

READ KEY DATA (A2.0.4)

The Key Data listed in Section 5.2.2.3 are read from the Key Data storage location and made available for use in "Preprocess Müller Matrix Elements (A2.1)". Some key data require basic preprocessing due to different conventions used by the key data provider and in this document. This preprocessing is done here as follows.

1. Correction factor *C* for azimuth and elevation angle dependence of irradiance response:

In the calibration key data, azimuth angles ϕkey are given relative to a "nominal" solar azimuth φ_{nom} = 325.0°. Convert φ_{key} to the Satellite Relative Actual Reference Coordinate System by adding φ_{nom}: $\varphi_{sat} = \varphi_{key} + \varphi_{nom}$.

In the calibration key data, the azimuth/elevation grid used for *C* is irregular. A regular grid is constructed as shown in Figure 6:

- Change the sign of the solar elevation angles *e* provided in the calibration key data file *BSDF_AIRR* to account for the different convention used during the on-ground calibration and characterisation activities.
- Discard those azimuth angles where *C* is given for elevation zero only.
- Discard those elevation angles where *C* is given for not more than two azimuth angles. N_e is the remaining number of elevation angles.
- For each remaining elevation angle *e* at each spectral point *i*,*j*, calculate the correction factors corresponding to φ_{nom} as arithmetic mean from the two azimuth angles closest to ϕ_{nom}. (These angles should be $\varphi_{nom} - \delta$ and $\varphi_{nom} + \delta$, δ depending on the elevation but smaller than 0.2°, so that the averaged correction factor indeed corresponds to φ_{nom}.): $C(e, \varphi_{nom})_{ij} = (C(e, \varphi_{nom} - \delta)_{ij} + C(e, \varphi_{nom} + \delta)_{ij})/2$.
- For the other remaining azimuth angles (remaining after the first step, but without $\varphi_{nom} - \delta$ and $\varphi_{nom} + \delta$), use *C* as given in the calibration key data. N_φ is the remaining number of azimuth angles.

In the example shown in Figure 6, $N_\varphi = 5$, and $N_e = 5$.

2. Wavelength calibration polynomial coefficients

Wavelength calibration polynomial coefficients in the calibration key data refer to pixel numbers *i* between 0 and 1023. However, the GOME-2 processor uses coefficients for normalised pixels *i* / 1023, see Equation 75. Therefore, the reference coefficients from the key data have to be adapted to the normalised pixels as follows:

$$a_{\text{ref},jm} = 1023^m A_{\text{ref},jm} \qquad (j = 1\ldots B,\ m = 0\ldots M)$$ *Equation 1*

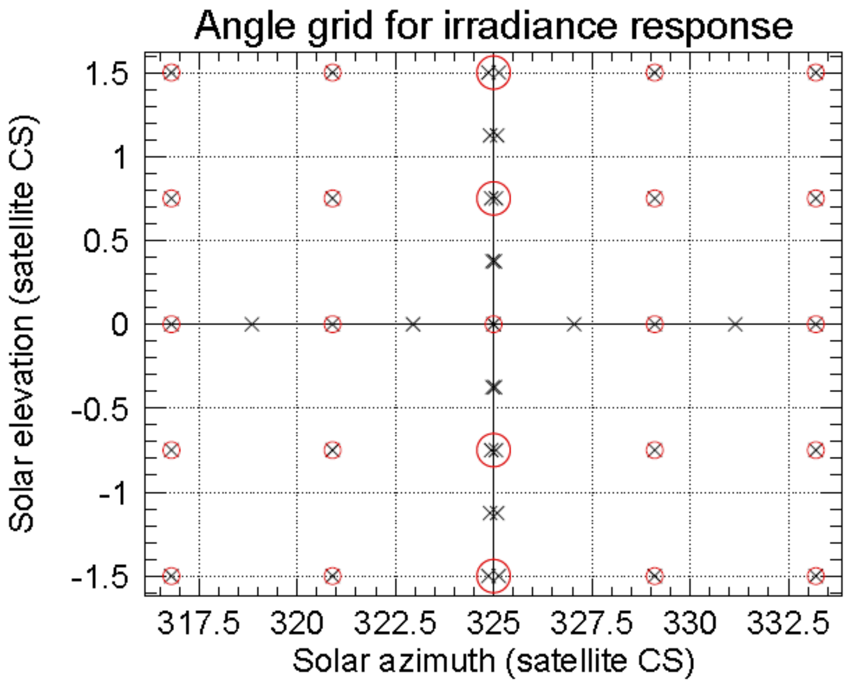

Figure 9: *Selection of azimuth/elevation angle pairs from the calibration key data describing the correction factor C for the angular dependence of the irradiance sensitivity. Solar azimuth angles have already been converted to the Satellite Actual Reference Coordinate System. The irregular grid provided in the key data is indicated by crosses. The processor uses only the data marked by circles. For the values indicated by large circles, pairs of measurements are averaged and assigned to the averaged azimuth angle.*

READ CORRECTION FACTOR DATA (A2.0.5)
The Correction Factor Data listed in Section 5.2.2.3 are read from the Key Data storage location and made available for use in Preprocess Müller Matrix Elements (A2.1).

READ IN-FLIGHT CALIBRATION DATA (A2.0.6)

The In-flight Calibration Data listed in Section 5.2.2.3 are read from the In-flight Calibration Data storage location and made available for use in Level 0 to 1a Processing (A2). If any of these datasets are no longer within the valid time range as specified in the initialisation parameters old_{Dark} , old_{PPG} , $old_{Spectral}$, old_{Etalon} or old_{SMR} , the processing shall continue using these data, a report shall be raised via the MCS and the products shall be flagged as degraded using the fields DEGRADED_PROC_MDR and PCD_BASIC F_OLD_CAL_DATA in the level 1a and 1b products as specified in [AD5].

READ LEVEL 0 INPUT DATA, SEPARATE SCANS AND GENERATE PCDS (A2.0.7)

The level 0 data stream or product is read and made available for use in Level 0 to 1a Processing (A2). The data stream or product is split into individual scans each comprising a maximum of 16 data packets. The first data packet in a complete scan is indicated by a data packet subset counter of zero, $sub = 0$. The last data packet in a scan is indicated by a data packet subset counter of 15, $sub = 15$. The data packet subset counters of intervening data packets are incremented by 1 per data packet. If one or more of the data packets within a valid scan are missing ($0 < N_{miss} < 16$ where N_{miss} is equal to the number of missing values in the sequence 0…15 of the data packet subset counters) then a flag, assumed to be initialised to 0 for all scans, is raised as follows:

$$F_{miss} = 1$$ *Equation 2*

The total number of missing data packets is incremented as follows:

$$N_{miss\_dp} = N_{mis\_dp} + N_{miss}$$ *Equation 3*

The total number of valid scans having missing data packets is incremented as:

$$N_{val\_dp} = N_{val\_dp} + F_{miss}$$ *Equation 4*

The number of missing scans may be determined from the data packet sequence control and the data packet sub-set counter. The total number in the product is calculated for $k = 1...N_{scan}$ as follows:

$$N_{miss\_scan} = N_{miss\_scan} + int((seq_{k,1} - sub_{k,1} - seq_{k-1,1} + sub_{k-1,1})/16) - 1$$ *Equation 5*

where the subscript 1 indicates the first received data packet in the scan. When $k = 1$, $k - 1$ indicates the last scan in the previous product.

Spectral band definitions (start pixel and number of pixels) are read from the first scan in the level 0 data stream or product. Relevant numbers in the science data packet are "channel 1 + 2 band separation" and PMD block B start and number of pixels. For PMD blocks CDE (bands 7 and 8) the number of pixels shall be set to 256.

5.2.3 Preprocess Müller Matrix Elements (A2.1)

USES GENERIC SUB-FUNCTIONS
Apply Spectral Calibration (AG.14)

USES AUXILIARY SUB-FUNCTIONS
Akima Interpolation (AX.4)

DATA GRANULE
Calibration Key Data

5.2.3.1 Objectives

To calculate the Müller Matrix elements, their ratios and relative errors from the Calibration Key Data.

5.2.3.2 Description

The following algorithms describe the calculation of the Müller Matrix elements (see Appendix E.2) from the Calibration Key Data. The Calibration Key Data are interpolated onto a common fixed wavelength grid before calculation of the MMEs begins. The calculation of MMEs is done once only as a pre-processing step before the processing of measurement data starts. The MMEs are corrected with M-factors which account for the in-flight degradation of instrument behaviour. When new correction factor data become available, the new M-factors must be applied to the precalculated MMEs but the MMEs themselves need not be recalculated. The update in usage of the newly corrected MMEs occurs at the start of processing a complete product. Those MMEs which are also needed for the Level 1a to 1b processing are output to the Level 1a product, together with their errors.

The parameters describing the polarisation sensitivity of the instrument are the ratios of Müller matrix elements M^2 and M^3 to M^1. Element M^1 itself describes the efficiency or '(ir)radiance response' of the instrument for unpolarised light. These ratios are needed both for the main detector channels and PMDs. In this section interpolation to the fixed wavelength grid and to a fine grid of scan and solar azimuth and elevation angles is carried out using Akima Interpolation (AX.4). This enables a faster Linear Interpolation (AX.2) or Spline Interpolation (AX.3) to be used at the point in the processing when the MMEs are interpolated to the exact wavelengths and angles required.

The error calculations presented in Section 5.2.3.4 describe relative errors in the MMEs. To obtain absolute errors they must be scaled by the measurement to which the MMEs are being applied at the point in the processing where they are used. It is assumed that the errors are not dependent on viewing angle and that errors in calibration at one viewing angle are independent of those at another. Errors in correction factors are assumed to be small with respect to errors in the on-ground radiance calibration. The error applicable to trace gas retrievals, carried out during level 1 to 2 processing, is the error in the *Sun-normalised radiance*. Since the radiance response and the irradiance response contain common errors, which cancel when the measured Earth-shine spectrum is divided by the measured solar spectrum, it is necessary to calculate the error in the sun-normalised radiance during the level 0-1 processing and include it in the product for users of the sun-normalised radiance level 1 data product.

Note: As pre-process, Müller Matrix Elements (A2.1) does not require any orbit, static auxiliary, in-flight calibration or level 0 data, it may be carried out independently of and in parallel to Read Orbit and Time Correlation Data (A2.0.2), Read Static Auxiliary Data (A2.0.3), Read In-flight Calibration Data (A2.0.6), Read Level 0 Input Data, Separate Scans and Generate PCDs (A2.0.7), as a pre-processing step. The MMEs and their errors need only be recalculated when new correction factor data is made available for use in Level 0 to 1a Processing (A2).

5.2.3.3 Variables

Variables are defined in the tables that follow:

5.2.3.3.1 Local Variables

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
ψ_s^{eq}	Viewing angle which is equivalent to the scan mirror angle when viewing the internal diffuser plate. Note that calibration key data are measured only for view angles outside the instrument. When viewing inside the instrument an equivalent angle must be used.	d	degrees	–	t	
$K_{\psi_s^{eq}}$	Viewing angle dependence of radiance response function for the specific viewing angle ψ_s^{eq}	d[D,B]	–	–	t	
$\chi_{\psi_s^{eq}}$	Viewing angle dependence of η, α and β for the specific viewing angle ψ_s^{eq}	d[D,B]	–	–	t	
$\delta\lambda_{MME}$	Sampling interval for Müller Matrix Element wavelength grid	d[B]	nm	–	t	

5.2.3.3.2 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
irrad_flag	Flag to determine which method is to be used for calculation of MMEs for irradiance	enum	–	i	A2.0.1	1 = end-to-end 2 = component
f_{I_R}	Scaling factor for calculation of error in sun-normalised radiance	d	–	i	A2.0.1	
$\lambda_{MME,\ start}$	Start wavelength for Müller Matrix Element wavelength grid	d[B]	nm	i	A2.0.1	
$\lambda_{MME,\ end}$	End wavelength for Müller Matrix Element wavelength grid	d[B]	nm	i	A2.0.1	
$N_{\psi f}$	Number of viewing angles for which the fine viewing angle grid is specified	w	–	i/o	A2.0.1/ A2.23.3	**GIADR-1a-MME** MME_N_PSI_F
N_{ef}	Number of solar elevation angles for which the fine elevation angle grid is specified	w	–	i/o	A2.0.1/A2.23.3	**GIADR-1a-MME** MME_N_E_F
$N_{\varphi f}$	Number of solar azimuth angles for which the fine azimuth angle grid is specified	d[N φ f]	–	i/o	A2.0.1/A2.23.3	**GIADR-1a-MME** MME_N_PHI_F

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
ψ_f	Viewing angles which define the fine viewing angle grid	$d[N_{\psi f}]$	degree	i/o	A2.0.1/A2.23.3	**GIADR-1a-MME** MME_PSI_F
e_f	Solar elevation angles which define the fine elevation angle grid	$d[N_{ef}]$	degree	i/o	A2.0.1/A2.23.3	**GIADR-1a-MME** MME_E_F
φ_f	Solar azimuth angles which define the fine azimuth angle grid	$d[N_{\varphi f}]$	degree	i/o	A2.0.1/A2.23.3	**GIADR-1a-MME** MME_PHI_F
ψ_s	Viewing angle for viewing the internal diffuser plate	d	degree	i/o	A2.0.1/A2.23.3	
$\psi_{SM,0}$	Viewing angle at $n_{SM} = 0$	d	degree	i/o	A2.0.1	
UseZeta	Flag indicating whether to use ζ key data to calculate μ^3. If set to false, μ^3 defaults to 0, which means the U polarisation component will not be considered in the polarisation correction.				A2.0.1	0 = do not use ζ 1 = use ζ (default)

5.2.3.3.3 Input from key dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
N_ϕ	Number of viewing angles for which calibration key data are measured	w	–	i	A2.0.4	
N_e	Number of solar elevation angles selected from calibration key data	w	–	i	A2.0.4	Keydata may contain more angles. N_e is the number of selected angles.
N_φ	Number of solar azimuth angles selected from calibration key data	w	–	i	A2.0.4	Keydata may contain more angles. N_φ is the number of selected angles.
ψ	Viewing angles for which calibration key data are measured	$d[N_\psi]$	degree	i	A2.0.4	
e	Solar elevation angles for which calibration key data are measured	$d[N_e]$	degree	i	A2.0.4	
φ	Solar azimuth angle for which calibration key data are	$d[N_\varphi]$	degree	i	A2.0.4	

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
	measured					
λ_{OL}	Wavelength of main channel separation (50% / 50% intensity point)	d[3]	nm	i	A2.0.4	

5.2.3.3.4 Input key dataset describing polarisation sensitivity

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
η^n	Intensity ratio, s-polarised to p-polarised light, for exact nadir direction	d[D,B]	–	i	A2.0.4	
ζ^n	Intensity ratio, –45° to +45° polarised light, for exact nadir direction	d[D,B]	–	i	A2.0.4	Only used if *UseZeta* = 1
α^n	Sensitivity ratio of PMD-s to PMD-p for s and p polarised light respectively, for exact nadir direction	d[D]	–	i	A2.0.4	
β^n	Normalised sensitivity of PMD-p to s-polarised light, for exact nadir direction	d[D]	–	i	A2.0.4	
γ	Normalised sensitivity of PMD-s to p-polarised light. Note that as the normalisation is with respect to the sensitivity of PMD-p to p-polarised light, this quantity is not dependent on scan angle.	d[D]	–	i	A2.0.4	
χ	Viewing angle dependence of η, α and β with respect to nadir	d[D,B, Nψ]	–	i	A2.0.4	
χ_ζ	Viewing angle dependence of ζ with respect to nadir	d[D,B, Nψ]	–	i	A2.0.4	
ε_η^n	Relative error in intensity ratio, s-polarised to p-polarised light, for exact nadir direction	d[D,B]	–	i	A2.0.4	
ε_χ	Relative error in viewing angle dependence of η, α and β with respect to nadir	d[D,B]	–	i	A2.0.4	

5.2.3.3.5 Input key dataset describing radiance sensitivity

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References
Ru n	Radiance response function for unpolarised light and exact nadir direction	d[D,B]	$BU.s^{-1}/(W.srcm^{3})$	i	A2.0.4	
κ	Viewing angle dependence of radiance response function			i	A2.0.4	
ε_Ru n	Relative error in radiance response function for unpolarised light and exact nadir direction			i	A2.0.4	
ε_κ	Relative error in viewing angle dependence of radiance response function			i	A2.0.4	

5.2.3.3.6 Input key dataset describing irradiance sensitivity

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References
I_u^0	Irradiance response function for zero elevation and azimuth angles	d[D,B]	$BU.s^{-1}/(W.srcm^{3})$	i	A2.0.4	
C	Correction factor for azimuth and elevation angle dependence of irradiance response	d[D,B,Ne,Nφ]	–	i	A2.0.4	After constructing a regular azimuth/ elevation grid
*BSDF*_s	BSDF of calibration unit in response to s-polarised light	d[D]	–	i	A2.0.4	
BSDF_p	BSDF of calibration unit in response to p-polarised light	d[D]	–	i	A2.0.4	
$\varepsilon\_I_u^0$	Relative error in irradiance response function for zero elevation and azimuth angles	d[D]	–	i	A2.0.4	
ε_*C*	Relative error in correction factor for azimuth and elevation angle dependence of irradiance response	d[D]	–	i	A2.0.4	
ε_*BSDF_p*	Relative error in BSDF of calibration unit in response to p-polarised light	d[D]	–	i	A2.0.4	
ε_*BSDF*_s	Relative error in BSDF of calibration unit in response to s-polarised light	d[D]	–	i	A2.0.4	

5.2.3.3.7 Input from correction factor dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
m	M-factor appropriate to the light path of the earth shine measurements	d[D,B]	–	i	A2.0.5	*default value 1.0 at the beginning of the in-orbit life of GOME-2*
m_cu	M-factor appropriate to the light path of the solar measurements, including the calibration unit	d[D,B]	–	i	A2.0.5	*default value 1.0 at the beginning of the in-orbit life of GOME-2*
λ^{mfac}	Wavelength grid on which m-factors are supplied	d[D,B]	nm	i	A2.0.5	

5.2.3.3.8 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
λ^{MME}	Wavelength grid on which the Müller Matrix Elements will be calculated	d[D,B]	nm	o	A2.23.3	**GIADR-1a-MME** MME_WL
M^1	Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D,B,$N_{\psi f}$]	BU.s^{-1}/(photons/(s.cm^2.s r.nm))	o	A2.23.3	**GIADR-1a-MME** MME_RAD_RESP
$M^{1,irrad}$	Müller matrix element describing the irradiance response of the instrument to unpolarised light	d[D,B,N_{ef},$N_{\varphi f}$]	BU.s^{-1} /(photons/(s.cm^2.n m))	o	A2.20, A2.23.3	**GIADR-1a-MME** MME_IRRAD_RESP
μ^2	Ratio of MMEs M^2 to M^1 describing the polarisation sensitivity of the instrument with respect to the Q Stokes component (s/polarisation). Derived from key data parameter η.	d[D,B, $N_{\psi f}$]	–	o	A2.21, A2.23.3	**GIADR-1a-MME** MME_POL_SENS
μ^3	Ratio of MMEs M^3 to M^1 describing the polarisation sensitivity of the instrument with respect to the U Stokes component	d[D,B, $N_{\psi f}$]	–	o	A2.21, A2.23.3	**GIADR-1a-MME** MME_POL_SHIFT

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
	(+/–45° polarisation). Derived from key data parameter.					
$M^1_{(s/p)\psi f}$	Response ratio of PMD-s/PMD-p as a function of viewing angle	d[D,$N_{\psi f}$]	–			
ε_M^1	Relative error in the Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D,B]	–	o	A2.21, A2.23.3	**GIADR-1a-MME** MME_ERR_RAD_ RESP
$\varepsilon\_M^{1,irrad}$	Relative error in the Müller matrix element describing the irradiance response of the instrument to unpolarised light	d[D,B]	–	o	A2.21, A2.23.3	**GIADR-1a-MME** MME_ERR_IRRAD_RESP
ε_μ^2	Relative error in the ratio of MMEs M^2 to M^1 which describes the polarisation sensitivity of the instrument with respect to the Q Stokes component	d[D,B]	–	o	A2.21, A2.23.3	**GIADR-1a-MME** MME_ERR_POL_SENS
ε_μ^3	Relative error in the ratio of MMEs M^3 to M^1 which describes the polarisation sensitivity of the instrument with respect to the U Stokes component	d[D,B]		o	A2.21, A2.23.3	**GIADR-1a-MME** MME_ERR_POL_SHIFT
$\varepsilon\_M^1_{SN}$	Relative error in the sun-normalised radiance response	d[D,B]		o	A2.21, A2.23.3	**GIADR-1a-MME** MME_SNRR_ERR

5.2.3.4 Algorithm

In case key data given for main channels have to be used for PMD channels: this is the case for the viewing angle dependencies κ, χ and $\chi\zeta$ – they have to be merged into a continuous wavelength grid by concatenating them at the overlap wavelengths λ_{OL}. This is similar to Step 8 in Section 5.2.16.4.2.

5.2.3.4.1 Perform Wavelength Interpolation of Calibration Key Data (A2.1.1)

First calculate the fixed wavelength grid λ^{MME} on which the MMEs will be calculated. In this section, assume D_j = 1024 for the main channels (j = 1…4) and D_j = 279 for the PMD channels (j = 5…6). This gives a total of 4654 grid points in line with the MME record defined in [AD5].

For $i = 0...D_j - 1$ and $j = 1...B$ calculate as follows:

$$\lambda_{ij}^{MME} = \lambda_{start,j}^{MME} + i \cdot \delta\lambda_j^{MME} \text{ where } \delta\lambda_j^{MME} = \frac{\lambda_{end,j}^{MME} - \lambda_{start,j}^{MME}}{D_j - 1} .$$

Equation 6

The Calibration Key Data are each supplied on a specific wavelength grid. Before being used to calculate the MMEs they (and their errors) are interpolated to the common wavelength grid λ^{MME} using Akima Interpolation (AX.4). The data should not be extrapolated. For those values of λ^{MME} which are outside the wavelength range of the Calibration Key data provided, the Calibration Key data at the end points of the wavelength range should be used. All subsequent calculations are assumed to be on the common wavelength grid.

5.2.3.4.2 Convert Key Data To MMEs (A2.1.2)

5.2.3.4.3 Polarisation Sensitivity (A2.1.2.1)

The conversion from Calibration Key Data which describes the polarisation sensitivity of the instrument to ratios of Müller matrix elements is for $i = 0...D_j - 1$, and $\psi = \psi_1 ... \psi_{N\psi}$:

Main channels ($j = 1...4$):

$$\mu_{ij,\,\psi}^2 = \frac{\eta_{ij}^n \cdot \chi_{ij,\,\psi} - 1}{\eta_{ij}^n \cdot \chi_{ij,\,\psi} + 1}$$

Equation 7

PMD p ($j = p$):

$$\mu_{ip,\,\psi}^2 = \frac{\beta_i^n \cdot \chi_{i,\,\psi} - 1}{\beta_i^n \cdot \chi_{i,\,\psi} + 1}$$

Equation 8

PMD s ($j = s$):

$$\mu^2_{is,\,\psi} = \frac{\alpha^n_i \cdot \chi_{i,\,\psi} - \gamma_i}{\alpha^n_i \cdot \chi_{i,\,\psi} + \gamma_i}$$ *Equation 9*

The radiance response ratio of the PMD channels is calculated as follows:

$$M^1_{(s/p)i,\,\psi} = \frac{\alpha^n_i \cdot \chi_{i,\,\psi} + \gamma_i}{\beta^n_i \cdot \chi_{i,\,\psi} + 1}$$ *Equation 10*

where $\chi_{i,\psi} = \chi_{ip,\psi} = \chi_{is,\psi}$ describes the scan angle dependence of α, β, and η.

The sensitivity towards the U polarisation component is for all channels (j = 1…4, p, s):

$$\mu^3_{ij,\,\psi} = \frac{\zeta^n_{ij} \cdot \chi_{\zeta i,\,\psi} - 1}{\zeta^n_{ij} \cdot \chi_{\zeta i,\,\psi} + 1} \text{ if } UseZeta = 1,$$ *Equation 11*

where $\chi_{\zeta i,\psi} = \chi_{\zeta ip,\psi} = \chi_{\zeta is,\psi}$ describes the scan angle dependence of ζ, and

$$\mu^3_{ij,\,\psi} = 0 \text{ for all scan angles if } UseZeta = 0.$$ *Equation 12*

5.2.3.4.3.1 RADIANCE SENSITIVITY (A2.1.2.2)

The matrix element M^1 which describes the efficiency or radiance response of the instrument to unpolarised light is calculated for $i = 0...D_j - 1$, $j = 1...B$ and $\psi = \psi_1...\psi_{N\psi}$ as:

$$M^1_{ij,\,\psi} = R^n_{u,\,ij} \cdot \kappa_{ij,\,\psi}$$ *Equation 13*

This expression applies both to main channel detectors and polarisation detectors.

5.2.3.4.3.2 IRRADIANCE SENSITIVITY (A2.1.2.3)

For irradiance sensitivity, the matrix element which describes the efficiency of the instrument for unpolarised light via the internal diffuser plate may be calculated using two different methods. A flag on the initialisation data will indicate which method shall be used.

- If *irrad_flag* = 1 then irradiance sensitivity based on end-to-end measurements of the irradiance response is calculated for i = $0...D_j - 1$, $j = 1...B$, $e = e_1...e_{Ne}$ and $\varphi = \varphi_1... \varphi_{N\varphi}$

$$M^{1,\,irrad}_{ij,\,e\varphi} = I^0_{u,\,ij} \cdot C(e,\varphi)_{ij}$$ *Equation 14*

- If *irrad_flag* = 2 then first calculate ψ^{eq}_s as

$$\psi^{eq}_s = |2 \cdot \psi_{SM,\,0}| - \psi_s \cdot$$ *Equation 15*

Then for $i = 0...D_j - 1$, $j = 1...B$ calculate $\kappa_{ij,\,\psi^{eq}}$ and $\chi_{ij,\psi^{eq}}$ by Spline Interpolation (AX.3) from $\kappa_{ij,\psi}$ and $\chi_{ij,\psi}$ respectively.

Then, the irradiance sensitivity based o polarisation sensitive measurements of the calibration unit (CU), combined with the radiance response of the instrument (without CU) is calculated for $i = 0...D_j - 1$, $e = e_1...e_{Ne}$ and $\varphi_1... \varphi_{N\varphi}$ as follows:

Main channels (j = 1...4):

$$M^{1,\,irrad}_{ij,\,e\varphi} = R^n_{u,\,ij} \cdot \frac{2 \cdot \kappa_{ij,\,\psi^{eq}_s}}{1 + \eta^n_{ij} \cdot \chi_{ij,\,\psi^{eq}_s}} \cdot (BSDF\_p_{ij} + \eta^n_{ij} \cdot \chi_{ij,\,\psi^{eq}_s} \cdot BSDF\_s_{ij}) \cdot C(e,\varphi)_{ij} \cdot$$ *Equation 16*

PMD p ($j = p$):

$$M^{1,\,irrad}_{ip,\,e\varphi} = R^n_{u,\,ip} \cdot \kappa_{ip,\,\psi^{eq}_s} \cdot BSDF\_p_{ip} \cdot C(e,\varphi)_{ip}$$ *Equation 16a*

PMD s ($j = s$):

$$M^{1,\,irrad}_{is,\,e\varphi} = R^n_{u,\,is} \cdot \kappa_{is,\,\psi^{eq}_s} \cdot BSDF\_s_{is} \cdot C(e,\varphi)_{is}$$ *Equation 16b*

5.2.3.4.4 Convert Units (A2.1.3)

It is necessary to convert M^1 and $M^{1\,irrad}$ from (BU/s)/(W.cm^{-3}.sr^{-1}) and (BU/s)/(W.cm^{-3}) to(BU/s)/(photons/(s.cm^2.nm.sr)) and (BU/s)/(photons/(s.cm^2.nm)). Therefore for $i = 0...D_j - 1$, $j = 1...B$, $\psi = \psi_1... \psi_{N\psi}$, $e = e_1...e_{Ne}$, and $\varphi_1... \varphi_{N\varphi}$ calculate:

$$M^{1}_{ij,\,\psi} = M^{1}_{ij,\,\psi} / (5.035 \times 10^{8} \cdot \lambda^{MME}_{ij})$$ *Equation 17*

$$M^{1,\,irrad}_{ij,\,e\varphi} = M^{1,\,irrad}_{ij,\,e\varphi} / (5.035 \times 10^{8} \cdot \lambda^{MME}_{ij})$$ *Equation 18*

5.2.3.4.5 Interpolate to Fine Grids (A2.1.4)

The MMEs describing polarisation sensitivity and radiance response of the instrument, M^1, M_s^1/M_p^1, μ^2 , μ^3, , and are interpolated from the viewing angles ψ to a fine grid of viewing angles ψ_f using Akima Interpolation (AX.4). The MMEs describing irradiance sensitivity $M^{1,irrad}$ are interpolated to fine grids of solar azimuth φ_f and elevation e_f using Akima Interpolation (AX.4).The interpolation to the fine grid of solar azimuth φ_f should be the first of the two interpolation operations. No extrapolation in angle shall be performed: An error shall be raised if any of the fine grid angles is outside the range covered by the angles from the key data.

5.2.3.4.6 Apply M-factors (A2.1.5)

Interpolate the m-factors from the wavelength grid associated with the m-factor data λ^{mfac} to the common wavelength grid, λ^{MME} , using Akima Interpolation (AX.4)

Apply the interpolated m-factors to the MMEs for $i = 0...D_j - 1$, $j = 1...B$, $\psi = \psi_1... \psi_{N\psi}$, $e = e_1...e_{Ne}$, and $\varphi_1... \varphi_{N\varphi f}$ as:

$$M^{1}_{ij,\,\psi} = M^{1}_{ij,\,\psi} / m_{ij}$$ *Equation 19*

$$M^{1,\,irrad}_{ij,\,e\varphi} = M^{1,\,irrad}_{ij,\,e\varphi} / (m_{ij} \cdot m\_cu_{ij})$$ *Equation 19a*

5.2.3.4.7 Calculate Errors on Müller Matrix Elements (A2.1.6)

5.2.3.4.7.1 Relative Errors for Radiance Response Parameters

The error in the calibrated radiance is calculated for $i = 0...D_j - 1$ and $j = 1...B$ as follows:

$$\varepsilon\_M^{1}_{ij} = \sqrt{[\varepsilon\_R^{n}_{u,\,ij}]^{2} + [\varepsilon\_\kappa_{ij}]^{2}}$$ *Equation 20*

5.2.3.4.7.2 Relative Errors for Irradiance Response Parameters

- If *irrad_flag* = 1 then for the end-to-end irradiance calibration method:

$$\varepsilon\_M_{ij}^{1,\,irrad} = \sqrt{[\varepsilon\_I_{u,\,ij}^{0}]^2 + [\varepsilon\_C_{ij}]^2}$$ *Equation 21*

- If *irrad_flag* = 2 then for the component level irradiance calibration method:

$$\varepsilon\_M_{ij}^{1,\,irrad} = \sqrt{[\varepsilon\_R_{u,\,ij}^{n}]^2 + [\varepsilon\_\kappa_{ij}]^2 + [(\varepsilon\_BSDF\_p_{ij} + \varepsilon\_BSDF\_s_{ij})/2]^2 + [\varepsilon\_C_{ij}]^2}$$ *Equation 21a*

- If *irrad_flag* = 1 then for the end-to-end irradiance calibration method, the relative error in MMES for the calculation of sun-normalised radiance is given by the following:

$$\varepsilon\_M_{SN,\,ij}^{1} = \sqrt{[f_{I\_R} \cdot \varepsilon\_I_{u,\,ij}^{0}]^2 + [\varepsilon\_C_{ij}]^2}$$ *Equation 22*

- If *irrad_flag* = 2 then for the component level irradiance calibration method, the relative error in MMEs for the calculation of sun-normalised radiance is given by:

$$\varepsilon\_M_{SN,\,ij}^{1} = \sqrt{[\varepsilon\_\kappa_{ij}]^2 + [(\varepsilon\_BSDF\_p_{ij} + \varepsilon\_BSDF\_s_{ij})/2]^2 + [\varepsilon\_C_{ij}]^2}$$ *Equation 23*

5.2.3.4.7.3 Relative Errors for Polarisation Sensitivity Parameters

The relative errors in ratios of Müller matrix elements are calculated for i = 0...*Dj* – 1 and *j* = 1...B, where $j \neq p$ and $j \neq s$ as in the following:

$$\varepsilon\_\mu_{ij}^{2} = \frac{\mathbf{2}[\eta_{ij}^{n}]^2}{(\eta_{ij}^{n})^2 - \mathbf{1}} \cdot \sqrt{[\varepsilon\_\eta_{ij}^{n}]^2 + [\varepsilon\_\kappa_{ij}]^2}$$ *Equation 24*

$$\varepsilon\_\mu_{ij}^{3} = \frac{\mathbf{2}[\zeta_{ij}^{n}]^2}{(\zeta_{ij}^{n})^2 - \mathbf{1}} \cdot \left|\varepsilon\_\zeta_{ij}^{n}\right|$$ *Equation 25*

5.2.4 Convert Housekeeping Data (A2.2)

Instrument Modes		*Instrument Data*	
Earth	√	PMD	
Dark	√	FPA	
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other	√		

Uses Generic Sub-Functions

Convert housekeeping data

Uses Auxiliary Sub-Function

None

Data Granule

One Scan

5.2.5 DETERMINE OBSERVATION MODE AND VIEWING ANGLES (A2.3)

Instrument Modes		*Instrument Data*	
Earth	√	PMD	
Dark	√	FPA	
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other	√		

Uses Generic Sub-Functions

Convert housekeeping data

Uses Auxiliary Sub-Function

None

Data Granule

One Scan

5.2.5.1 Objectives

Derive the observation mode, the viewing angles and the corresponding UTC times for a scan from a combination of housekeeping data

5.2.5.2 Description

Data from different observation modes will be sent to different branches of the 0 to 1b processing. This module derives the observation mode for a scan from a combination of housekeeping data and the scanner viewing angles. The viewing angles themselves are calculated from the scan mirror readings in the data packet. Scans which do not match any of the available observation modes are classified as “invalid”. Furthermore both the PMD transfer and readout mode are determined, and the UTC times corresponding to the scan mirror positions are calculated.

The observation modes for the GOME-2 instrument have been introduced in Section 2.3.3. Besides the routine earth observation modes, several in-flight calibration modes and instrument maintenance modes are available. The PMD readout and transfer modes are introduced in Appendix B.

Notes:

- Measurements from the six earth observation modes will be handled in the same way in subsequent processing up to level 1b. The distinction is however relevant for the PQE and SPA tools, and for processing to higher level products.
- This module does not check whether the scan is actually usable in the further processing. It is left to the modules processing the individual modes to exclude particular scans. For example, from the scans assigned to the sun (or moon) mode, only measurements where the sun (or moon) is actually within the field-of-view will be selected later on. For lamp modes, a stabilisation time will be allowed, etc.

5.2.5.3 Variables

5.2.5.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
k	Index number of current scan mirror readout within scan	i	–	t	–	$0 \ldots R_\psi - 1$ (R_ψ) See below for extra entry R_ψ
m	Subset (number of 375 ms ground pixel) within scan	i	–	t	–	0…15

5.2.5.3.2 Local Variables

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
M	Threshold for determining whether a SBT counter rollover has taken place in the time interval under consideration.	i	$2^{-16}s$	t	–	

5.2.5.3.3 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
$\psi_{SM,0}$	Viewing angle at $n_{SM} = 0$	d	degree	i	A2.0.1	
$\psi_{SM,1}$	Viewing angle increment per binary unit in n_{SM}	d	degree/BU	i	A2.0.1	
ψ_{EARTH}	Viewing angle range for earth view	d[2]	degree	i	A2.0.1	
ψ_{MOON}	Viewing angle range for moon view	d[2]	degree	i	A2.0.1	
ψ_{DARK}	Viewing angle range for dark view	d[2]	degree	i	A2.0.1	
ψ_{SLS}	Viewing angle range for SLS view	d[2]	degree	i	A2.0.1	
$\psi_{DIFFUSER}$	Viewing angle range for diffuser view	d[2]	degree	i	A2.0.1	
ψ_{WLS}	Viewing angle range for WLS view	d[2]	degree	i	A2.0.1	
ψ_{Nadir}	Forward scan centre viewing angle range for nadir view	d[2]	degree	i	A2.0.1	
ψ_{NorthP}	Forward scan centre viewing angle range for north polar view	d[2]	degree	i	A2.0.1	

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
ψ_{SouthP}	Forward scan centre viewing angle range for south polar view	d[2]	degree	i	A2.0.1	
$\psi_{Scan,min}$	Minimum viewing angle amplitude for a scan to be classified into one of the earth scanning modes	d	degree	i	A2.0.1	
I_{on}^{WLS}	Minimum WLS current for the WLS to be considered "on"	d	A	i	A2.0.1	
I_{on}^{SLS}	Minimum SLS current for the SLS to be considered "on"	d	A	i	A2.0.1	
Δt_{SM}	Offset in time of first scan mirror position in packet with respect to UTC time stamp in packet	d	s	i	A2.0.1	
t_{first}	First valid UTC time	d	fractional days	i	A2.0.1	
t_{last}	Last valid UTC time		fractional days	i	A2.0.1	
C	Number of on-board clock steps per step of SBT_0	i	–	i	A2.0.1	
N	Number of different values the SBT counter can assume.	i	–	i	A2.0.1	
f_{roll}	Fraction of full SBT counter range to consider for the rollover check.	i	–	i	A2.0.1	
UTCOption	Algorithm option to calculate UTC	enum	–	i	A2.0.1	
F_2	Scaling factor for UTC option 2	d	–	i	A2.0.1	
F_3	Scaling factor for UTC option 3	d	–	i	A2.0.1	

5.2.5.3.4 *Input/Output from other functions*

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
HK	Housekeeping data	w[16, 488]	–	i	A2.0.7	See note 1 below
nSM	Scan mirror resolved position	w[R ϕ]	BU	i	A2.0.7	sampled at 93.75 ms, part of *HK*
t	UTC time stamp in the Science Data Packet (see [AD9])	w[16,3]	days, 2^{16} ms, ms	i	A2.0.7	UTC option 1: sampled at 375 ms, part of *HK*. *HK* contain also a word for µs, this can be ignored.

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
s	SBT time stamp in the Science Data Packet (see [AD9])	w[16,3]	2^{16} s, s, 2^{-16} s	i	A2.0.7	UTC options 2 and 3: sampled at 375 ms, part of *HK*
T	UTC for time correlation in the Science Data Packet (see [AD9])	w[3]	days, 2^{16} ms, ms	i	A2.0.7	UTC option 2: sampled at 375 ms, use first packet in scan only, part of *HK*.
S	SBT for time correlation in the Science Data Packet (see [AD9])	w[3]	2^{16}s, s, 2^{-16}s	i	A2.0.7	UTC option 2: sampled at 375 ms, use first packet in scan only, part of *HK*.40-bit counter, highest 8 bits are always zero.
ΔT	Time increment for time correlation in the Science Data Packet (see [AD9])	w[2]	–	i	A2.0.7	UTC option 2: sampled at 375 ms, use first packet in scan only, part of *HK*
UTC_0	UTC for time correlation	d	fractional days	t *or* i	UTC option 3: A2.0.2	UTC option 2: calculated from *T*. UTC option 3: external information.
SBT_0	SBT for time correlation	d	2^{-16} s	t *or* i	UTC option 3: A2.0.2	UTC option 2: calculated from *S*. UTC option 3: external information.
T_s	Time increment for time correlation	d	–	t *or* i	UTC option 3: A2.0.2	UTC option 2: calculated from . UTC option 3: external information.
F_{nn_WLSU}	Flag indicating non-nominal WLS voltage in scan	bool	–	i	A2.2	
F_{nn_WLSI}	Flag indicating non-nominal WLS current in scan	bool	–	i	A2.2	
F_{nn_SLSU}	Flag indicating non-nominal SLS voltage in scan	bool	–	i	A2.2	
F_{nn_SLSI}	Flag indicating non-nominal SLS current in scan	bool	–	i	A2.2	

5.2.5.3.5 *Local Variable*

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
sbt	SBT	d	2^{-16} s	t		UTC options 2 and 3: calculated from *s*.

5.2.5.3.6 Global PCDs accumulated per product

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
N_{inv_UTC}	Number of scans with invalid UTC	w	–	g	A2.22	
N_{Nad_scan}	Number of scans in *Nadir_scan* observation mode	w	–	g	A2.22	
N_{Nth_scan}	Number of scans in *Nth_pole_scan* observation mode	w	–	g	A2.22	
N_{Sth_scan}	Number of scans in *Sth_pole_scan* observation mode	w	–	g	A2.22	
N_{Oth_scan}	Number of scans in *Other_scan* observation mode	w	–	g	A2.22	
N_{Nad_static}	Number of scans in *Nadir_static* observation mode	w	–	g	A2.22	
N_{Oth_static}	Number of scans in *Other_static* observation mode	w	–	g	A2.22	
N_{Dark}	Number of scans in *Dark* observation mode	w	–	g	A2.22	
N_{LED}	Number of scans in *LED* observation mode	w	–	g	A2.22	
N_{WLS}	Number of scans in *WLS* observation mode	w	–	g	A2.22	
N_{SLS}	Number of scans in *SLS* observation mode	w	–	g	A2.22	
N_{SLS_diff}	Number of scans in *SLS* over diffuser observation mode	w	–	g	A2.22	
N_{Sun}	Number of scans in *Sun* observation mode	w	–	g	A2.22	
N_{Moon}	Number of scans in *Moon* observation mode	w	–	g	A2.22	
N_{Idle}	Number of scans in *Idle* observation mode	w	–	g	A2.22	
N_{Test}	Number of scans in *Test* observation mode	w	–	g	A2.22	
N_{Dump}	Number of scans in *Dump* observation mode	w	–	g	A2.22	
$N_{Invalid}$	Number of scans assigned as *Invalid* observation mode	w	–	g	A2.22	

5.2.5.3.7 Local Variable

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
ψ	Scanner viewing angle with additional element at end of scan	$d[R_\psi+1]$	degree	o	A2.6, A2.21, A2.23.1	**MDR-1a-*** SCANNER_ ANGLE Earth and calibration modes only, one value per value of $n_{SM,k}$, one additional element at the end (see below)
t_ψ	UTC corresponding to scanner viewing angle with additional element at end of scan	d[Rψ+1]	days	o	A2.6	
mode	Observation mode	enum	–	o	various as well as A2.23.1	**MDR-1*** OBSERVATION_ MODE one enumerated value per scan
pmd_transfer	PMD transfer mode	enum	–	o	various as well as A2.23.1	**MDR-1*** PMD_TRANSFER one enumerated value per scan
pmd_readout	PMD readout mode	enum	–	o	various as well as A2.23.1	**MDR-1*** PMD_READOUT one enumerated value per scan
F_{inv_UTC}	Flag indicating invalid UTC in scan	bool	–	o	A2.23.1	**MDR-1*** PCD_BASIC F_INV_UTC 0 = valid UTC 1 = invalid UTC

Note: See below for the subset of HK data actually used and [AD9] for their location within HK. 16 data packets per scan, HK data are the first 488 words of a data packet.

5.2.5.4 Algorithm

5.2.5.4.1 Determine Observation Mode and Viewing Angles (A2.3.1)

Table 4 indicates the required values for selected housekeeping data per observation mode. For a scan to be assigned to a particular mode, **the relevant conditions must be fulfilled throughout the scan**. In particular, all R_ψ viewing angles within a scan must be within the range indicated in Table 4. For example, for a scan to be assigned to the earth observation category, we must have the following:

$$\psi_{EARTH,0} \leq \psi_k \leq \psi_{EARTH,1} \qquad (k = 0, \ldots, R_\psi - 1)$$ *Equation 26*

The viewing angle ranges relevant for classification into observation modes will be defined in the initialisation dataset. The values indicated in the variable list are based on instrument design and observation geometry.

Notes on individual columns in Table 4 (below) and links to [AD9]:

- PMD/FPA: "On" if status flags (ICU word 1) indicate SW status "normal", HW status "on", and (ICU word 4) "no calibration". Note that the cooler status (subsystem mode word 1) is not relevant here.
- Shutter: "Open" if corresponding status flag (subsystem mode word 1) indicates "open" and "motor off".
- WLS: "On" if WLS (QTH) status flag (ICU word 2) is set "on" and WLS current above I_{on}^{WLS} and WLS current and voltage are valid, i.e., neither of the flags F_{nn_WLSU} and F_{nn_WLSI} is set for the current scan.
- SLS: "On" if SLS (HCL) status flag (ICU word 2) is set "on" and SLS current above I_{on}^{SLS} and SLS current and voltage are valid, i.e., neither of the flags F_{nn_SLSU} and F_{nn_SLSI} is set for the current scan.
- LED: "On" if at least one of the four LED status bits (ICU word 2) is set "on".
- Scan unit: Scan unit status in subsystem mode word 2.
- Number of dumped words: This refers to SDP word 175, and *not* to word 184, the number of dumped words for the scan unit which is always > 0. (The layout of words 174–179 – reporting dump information – in issue 6 of [AD9] is no longer valid. This will be corrected in the next issue.)
- Test pattern: Flag in ICU word 4.

The scan is first checked to be in one of the modes test, dump, or idle (in this order).

If it has not been assigned to one of these three modes, the viewing angles ψ_k are derived from the scan mirror resolver readouts $n_{SM,k}$ as follows:

$$\psi_k = \psi_{SM,0} + \psi_{SM,1} n_{SM,k} \qquad (k = 0 \ldots R_\psi - 1).$$ *Equation 27*

The last viewing angle ψ_{64} is set to be the same as the first one:

$$\psi_{64} = \psi_0 \, .$$ *Equation 28*

This additional element will simplify the description later on (A2.6) for the calculation of geolocations for earth measurements.

Viewing angles and the relevant HK data are then used as follows to derive the observation mode:
It is checked whether the scan can be assigned to the earth observation category according to Table 4. If so, the earth observation mode is determined from the viewing angles at the start, middle, and end f the forward scan, ψ_0, ψ_{24}, and ψ_{48}:

• If ($|\psi_{48} - \psi_0| \geq \Psi_{scan,min}$, the earth mode belongs to one of the four scanning modes:
  nadir scanning, if $\psi_{Nadir,0} \leq \psi_{24} \leq \psi_{Nadir,1}$
  north polar scanning if $\psi_{NorthP,0} \leq \psi_{24} \leq \psi_{NorthP,1}$
  south polar scanning if $\psi_{SouthP,0} \leq \psi_{24} \leq \psi_{SouthP,1}$
  other scanning otherwise.

• Otherwise ($|\psi_{48} - \psi_0| < \psi_{scan,min}$), it belongs to one of the two static modes:
  nadir static, if $\psi_{Nadir,0} \leq \psi_{24} \leq \psi_{Nadir,1}$
  other static otherwise.

If the scan has not been assigned to the earth observation category, it is checked whether it can be assigned to one of the calibration modes according to Table 4.

If the scan has not been assigned to any of the calibration modes, it is assigned to invalid mode.

Earth Observation

Mode	*Viewing Angle Range*	*PMD/FPA*	*Shutter*	*WLS*	*SLS*	*LED*	*Scan Unit*	*Dumped Words*	*Test Pattern*
nadir scanning	ψ_{EARTH}	on	closed	off	off	off	on/normal	0	no
north polar scanning	See text for assignment to individual modes								
other scanning									
nadir static									
other static									

Calibration

Mode	*Viewing Angle Range*	*PMD/FPA*	*Shutter*	*WLS*	*SLS*	*LED*	*Scan Unit*	*Dumped Words*	*Test Pattern*
dark	ψ_{DARK}	on	closed	off	off	off	On/normal	0	no
sun	$\psi_{DIFFUSER}$	on	open	off	off	off	On/normal	0	no
WLS	ψ_{WLS}	on	closed	on	off	off	On/normal	0	no

SLS direct	ψ_{SLS}	on	closed	off	on	off	On/normal	0	no
SLS via diffuser	$\psi_{DIFFUSER}$	on	closed	off	on	off	On/normal	0	no
LED	ψ_{DARK}	on	closed	off	off	on	On/normal	0	no
moon	ψ_{MOON}	on	closed	off	off	off	On/normal	0	no

Other

Mode	*Viewing Angle Range*	*PMD/FPA*	*Shutter*	*WLS*	*SLS*	*LED*	*Scan Unit*	*Dumped Words*	*Test Pattern*
idle	N/A	N/A	N/A	N/A	N/A	N/A	off or on/init	N/A	N/A
dump	N/A	N/A	N/A	N/A	N/A	N/A	N/A	> **0**	N/A
test	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	**yes**
invalid	N/A The scan cannot be assigned to any of the modules above.								

Table 4: Housekeeping data settings per observation mode

5.2.5.4.2 Determine UTC Time Grid (A2.3.2)

For geolocating the GOME-2 measurements (A2.6), the UTC time corresponding to each scanner viewing angle has to be known. There are three options for assigning a UTC time to a packet. The selection is via a parameter in the initialisation file.

UTC option 1: Use the UTC time given in the packet. The UTC time t is given once per Science Data Packet, i.e., 16 times per scan, in four words per packet, the first three denoting the days since 1 Jan 2000 ($t_{m,0}$) and the milliseconds of the day (high word: $t_{m,1}$, low word: $t_{m,2}$). Within each packet, the first scanner position is given at time Δt_{SM} (in seconds) relative to the UTC time stamp t.

Therefore, the times corresponding to the first scanner readout per packet are set to the following:

$$t_{\psi,4m} = t_{m,0} + (2^{16} \cdot t_{m,1} + t_{m,2} + 1000 \cdot \Delta t_{SM}) / (\text{number of ms per day}) \quad (m = 0 \ldots 15)$$ *Equation 29*

UTC option 2: Calculate the UTC time from the SBT and the time correlation information given in the packet. Use the time correlation parameters UTC_0, SBT_0, and T_s given in the science data packet. Like the UTC in option 1, UTC_0 is given in four words per packet. Only the values from the first packet in the scan are used here. The first three words denote the days since 1 Jan 2000 (T_0) and the milliseconds of the day (high word: T_1, low word: T_2).

$$\mathrm{UTC}_0 = T_0 + (2^{16} \cdot T_1 + T_2) / (\text{number of ms per day}) \quad (m = 0 \ldots 15).$$ *Equation 30*

In the science data packet, sbt and SBT_0 are given in three words (six bytes), starting with the high word ($s_{m,0}$, S_0). Calculate them (in 2^{-16} seconds) by combining these words as follows:

$$\mathrm{sbt}_m = 2^{32} \cdot s_{m,0} + 2^{16} \cdot s_{m,1} + s_{m,2} \quad (m = 0 \ldots 15)$$ *Equation 31*

$$\mathrm{SBT}_0 = 2^{32} \cdot S_0 + 2^{16} \cdot S_1 + S_2$$ *Equation 32*

Next check whether there has been a rollover of the SBT counter between time *0* and time *m*.

First calculate the following:

$$\Delta\mathrm{SBT}_m = \mathrm{sbt}_m / C - \mathrm{SBT}_0 \text{ and } M = \frac{N}{f_{roll}}$$ *Equation 32a*

where C is a scaling factor required to accommodate the possibility of sbt_m and SBT_0 having different time resolutions which expresses the number of on-board clock steps per step of SBT_0. For UTC option 2, *C* has a default value of 1.

Then

$$\text{if } \Delta\mathrm{SBT}_m > M \text{ set } \Delta\mathrm{SBT}_m = \Delta\mathrm{SBT}_m - N \text{ and}$$ *Equation 32b*

$$\text{if } \Delta\mathrm{SBT}_m < -M \text{ set } \Delta\mathrm{SBT}_m = \Delta\mathrm{SBT}_m + N$$ *Equation 32c*

sbt and SBT_0 are 40-bit counters, i.e., the highest eight bits are always zero. The time increment T_s is given in two words (high word: ΔT_0, low word: ΔT_1):

Note: Therefore, the SBT counter wraps around every 2^{24} s, corresponding to somewhat more than 194 days.

$$T_s = 2^{16} \cdot \Delta T_0 + \Delta T_1$$ *Equation 33*

Finally, calculate the times corresponding to the first scanner readout per packet as follows:

$$t_{\psi,4m} = \mathrm{UTC}_0 + [\Delta\mathrm{SBT}_m \cdot T_s / F_2 + \Delta t_{SM}] / (\text{number of s per day}) \quad (m = 0 \ldots 15)$$ *Equation 34*

UTC option 3: Calculate the UTC time from the SBT and the time correlation information given as external parameters. Use the time correlation parameters UTC_0, SBT_0, and T_s given as external parameters. Calculate $\Delta\mathrm{SBT}_m$ using equation (31) and equation (32). Note that for UTC option 3, *C* has a default value of 256 for UTC.

Calculate the times corresponding to the first scanner readout per packet as follows:

$$t_{\psi,4m} = \mathrm{UTC}_0 + [\Delta\mathrm{SBT}_m \cdot T_s / F_3 + \Delta t_{SM}] / (\text{number of s per day}) \quad (m = 0 \ldots 15)$$ *Equation 35*

All UTC options: The remaining elements of t_ψ are extrapolated and interpolated as follows:

$$t_{\psi,64} = t_{\psi,60} + t_{\psi,60} - t_{\psi,56}$$ Equation 36

$$t_{\psi,k} = (t_{\psi,k-2} + t_{\psi,k+2})/2 \qquad (k = 2, 6, \ldots, 62)$$ Equation 37

$$t_{\psi,k} = (t_{\psi,k-1} + t_{\psi,k+1})/2 \qquad (k = 1, 3, \ldots, 63)$$ Equation 38

Assuming the UTC time stamps t are equally spaced (every 375 ms), we end up with an equidistant 93.75 ms time grid t_ψ corresponding to the scanner viewing angles ϕ. If for any of the t_ϕ, $t_\psi < t_{first}$ or $t_\psi > t_{last}$ or then set $t_\psi =$ undefined.

Note: Elements $t_{\psi,0}$ and $t_{\psi,64}$ will be used as record start and stop times for the Generic Record Header of the corresponding Measurement Data Record (see [AD5]).

5.2.5.4.3 Determine PMD Readout and Transfer Mode (A2.3.3)

The actual PMD readout and transfer modes are part of the HK data *HK*, and as such given per science data packet, i.e., 16 times per scan.

Determine PMD readout mode for the scan: If all 16 individual readout modes have the same value, assign this value to *pmd_readout*. Otherwise, assign a number (different from any of the valid readout modes) indicating invalid readout mode for the scan.

Determine PMD transfer mode for the scan: If all 16 individual transfer modes have the same value, assign this value to *pmd_transfer*. Otherwise assign a number (different from any of the valid transfer modes) indicating invalid transfer mode for the scan.

5.2.5.4.4 Determine PCDs from Observation Mode (A2.3.4)

All PCDs listed are valid for one scan. Global incremental counter variables are assumed to be initialised to zero at the beginning of processing a product. F_{inv_UTC} is also assumed to be initialised to zero for each scan.

- For all t_ϕ in the scan then if $t_\psi =$ undefined

$$F_{inv\_UTC} = 1 \text{ and } N_{inv\_UTC} = N_{inv\_UTC} + 1$$ Equation 39

- If *mode = Nadir_scan*

$$N_{Nad\_scan} = N_{Nad\_scan} + 1$$ Equation 40

- If *mode = Nth_pole_scan*

$$N_{Nth\_scan} = N_{Nth\_scan} + 1$$ Equation 41

- If *mode = Sth_pole_scan*

$$N_{Sth\_scan} = N_{Sth\_scan} + 1$$ Equation 42

If $mode = Other\_scan$

$$N_{Other\_scan} = N_{Other\_scan} + 1 \quad \text{Equation 43}$$

- If $mode = Nadir\_static$

$$N_{Nad\_static} = N_{Nad\_static} + 1 \quad \text{Equation 44}$$

- If $mode = Other\_static$

$$N_{Oth\_static} = N_{Oth\_static} + 1 \quad \text{Equation 45}$$

- If $mode = Dark$

$$N_{Dark} = N_{Dark} + 1 \quad \text{Equation 46}$$

- If $mode = LED$

$$N_{LED} = N_{LED} + 1 \quad \text{Equation 47}$$

- If $mode = WLS$

$$N_{WLS} = N_{WLS} + 1 \quad \text{Equation 48}$$

- If $mode = SLS$

$$N_{SLS} = N_{SLS} + 1 \quad \text{Equation 49}$$

- If $mode = SLS\_diff$

$$N_{SLS\_diff} = N_{SLS\_diff} + 1 \quad \text{Equation 50}$$

- If $mode = Sun$

$$N_{Sun} = N_{Sun} + 1 \quad \text{Equation 51}$$

- If $mode = Moon$

$$N_{Moon} = N_{Moon} + 1 \quad \text{Equation 52}$$

- If $mode = Idle$

$$N_{Idle} = N_{Idle} + 1 \quad \text{Equation 53}$$

- If $mode = Test$

$$N_{Test} = N_{Test} + 1 \quad \text{Equation 54}$$

- If $mode = Dump$

$$N_{Dump} = N_{Dump} + 1 \quad \text{Equation 55}$$

- If $mode = Invalid$

$$N_{Invalid} = N_{Invalid} + 1 \quad \text{Equation 56}$$

5.2.6 DETERMINE PCDS FROM RAW INTENSITY (A2.4)

Instrument Modes		***Instrument Data***	
Earth	√	PMD	√
Dark	√	FPA	√
Sun	√	Housekeeping	
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		

USES GENERIC SUB-FUNCTIONS

Check for Saturated Pixels (AG.6)

Check for Hot Pixels (AG.7)

USES AUXILIARY SUB-FUNCTIONS

None.

DATA GRANULE

One Scan

5.2.6.1 Objective

To apply generic saturation and hot pixel checks to the raw intensity. Saturation checks are applied to data from all measurement modes with the exception of PMD data transferred in *band + raw* or *band + mixed* mode. Hot pixel checks are applied only to data from *dark*, *LED* and *WLS* observation modes. The mean raw signal is also calculated for product quality monitoring purposes.

5.2.6.2 Description

Generic saturation and hot pixel checks are applied to the raw intensities. These checks are applied to all data including those that may later be excluded from the processing on the basis of subsequent quality checking. Only PMD data transferred in *band + raw* or *band + mixed* transfer mode are excluded from the checks.

Saturation checks are applied to data from all measurement modes on the basis of thresholds specified per channel in the initialisation dataset. If any detector pixels are found to be saturated in any readout within a scan, a flag is raised for the appropriate band of that scan. Furthermore, a saturation mask is generated per readout so that bands affected are excluded from further processing.

Hot pixel checks are applied only to those data which do not have large spectral variation i.e. data from *dark*, *LED* and *WLS* observation modes. Hot pixels are those whose intensities deviate from the intensity of neighbouring detector pixels by more than a given threshold, specified per channel and as a function of mode in the initialisation dataset. If any detector pixels are found to be hot in any readout within a scan, a flag is raised for the appropriate band of that scan. A hot pixel mask is also generated for each read out in the scan.

The mean raw signal per band is also calculated for product quality monitoring purposes.

5.2.6.3 Variables

5.2.6.3.1 *Input/ from initialisation dataset*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
t_{min}	Threshold for the minimum uncalibrated signal per band	w[B]	BU	i	A2.0.1	
t_{sat}	Saturation threshold per band	d[B]	BU	i	A2.0.1	
t_{hot}	Hot pixel threshold per band	d[B]	BU	i	A2.0.1	

5.2.6.3.2 *Input/output from other functions*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
mode	Observation mode	enum	-	i	A2.3	
pmd_transfer	PMD transfer mode	enum[N]	-	i	A2.3	
satpix	Saturation mask per band	b[B,R_{FPA}]	-	i/o	AG.6/AX.1 and various	1 = saturation 0 = no saturation
hotpix	Hot pixel mask	b[D,B,R_{FPA}]	-	i/o	AG.7/AX.1 and various	1 = normal 0 = hot

5.2.6.3.3 *Input from 1v0 data stream*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
S	Detector array readout values for which the saturated and hot pixel mask are being generated.	d[D,B]	BU	i	A2.07	

5.2.6.3.4 Global PCDs accumulated per product

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
Nsat	Number of scans with saturated pixels	w[B]	-	g	A2.22	
N_{hot}	Number of scans with hot pixels	w[B]	-	g	A2.22	
N_{min}	Number of scans where the minimum intensity of at least one pixel within a band is below a specified threshold per band	w[B]	-	g	A2.22	

5.2.6.3.5 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
Fsat	Flag indicating saturated pixels per band in scan	bool[B,RFPA]	–	i/o	AG.6/A2.23.1	**MDR-1*** PCD_BASICF_SAT 1 = saturation 0 = no saturation
F_{hot}	Flag indicating hot pixels per band in scan	bool[B,RFPA]	–	i/o	AG.7/A2.23.1	**MDR-1*** PCD_BASICF_HOT 1 = hot 0 = normal
F_{min}	Flag indicating that the uncalibrated signal for any pixel within a channel is below a specified threshold per band	bool[B,RFPA]	–	o	A2.23.1	**MDR-1*** PCD_BASICF_MIN 1 = below 0 = not below
$\bar{S}$	Mean raw signal per band	w[B]	BU	i/o	AG.7/A2.23.1	**MDR-1*** PCD_BASICMEAN_UC

5.2.6.4 Algorithm

- If *pmd_transfer* = *raw* (i.e. PMD data is transferred in raw mode) the following calculations are carried out for both main and PMD channels. Otherwise the calculations are carried out for main channels only. Nothing is done for PMD channels.
- Calculate the mean raw signal per band for $j = 1...B$ as:

$$\bar{S}_j = \sum_{i=0}^{D_j-1} S_{ij}/D_j \quad \text{Equation 57}$$

- F_{min} is assumed to be initialised to zero. Then for $i = 0...D_j - 1$, $j = 1...B$ and every readout k calculate:
  if $S_{ij} < t_{min,j}$ set $F_{min,jk} = 1$.

$$N_{min,\ j} = N_{min,\ j} + 1 \text{ (accumulated per channel and scan)} \quad \text{Equation 58}$$

- F_{sat} is assumed to be initialised to zero. Generate a saturation mask per band and a saturation flag using Check for Saturated Pixels (AG.6).
  N_{sat} is assumed to be initialised to zero at the start of processing a product so for all readouts k if any of $F_{sat,jk} = 1$

$$N_{sat,j} = N_{sat,\ j} + 1 \text{ (accumulated per channel and scan)} \quad \text{Equation 59}$$

- F_{hot} is assumed to be initialised to zero. If *mode = dark* or *mode = LED* or *mode = WLS* then generate a hot pixel mask and flag using Check for Hot Pixels (AG.7). N_{hot} is assumed to be initialised to zero at the start of processing a product so for all readouts k if any of $F_{hot,jk} = 1$

$$N_{hot,j} = N_{hot,j} + 1 \text{ (accumulated per channel and scan)} \quad \text{Equation 60}$$

Otherwise, for $i = 0...D_j - 1$, $j = 1...B$

$$hotpix_{ij} = 1 \quad \text{Equation 61}$$

5.2.7 Prepare PMD Data (A2.5)

Instrument Modes		***Instrument Data***	
Earth	√	PMD	√
Dark	√	FPA	
Sun	√	Housekeeping	
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other			

USES GENERIC SUB-FUNCTIONS

Prepare PMD Data (AG.4)

USES AUXILIARY SUB-FUNCTIONS

None.

DATA GRANULE

One Scan

5.2.8 CALCULATE GEOLOCATION FOR FIXED GRID (A2.6)

Instrument Modes		***Instrument Data***	
Earth	√	PMD	
Dark	√	FPA	
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other	√		

USES GENERIC SUB-FUNCTIONS

PGE services providing geolocation parameters will be used.
Initialise Orbit Propagator (AG.1)
Calculate Centre Coordinates (AG.19)

USES AUXILIARY SUB-FUNCTIONS

None

DATA GRANULE

One Scan

5.2.9 Determine PCDs from Geolocation (A2.7)

Instrument Modes		*Instrument Data*	
Earth	√	PMD	
Dark	√	FPA	
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other	√		

USES GENERIC SUB-FUNCTIONS

Check for SAA (AG.8)

Check for Sunglint (AG.9)

Check for Rainbow (AG.10)

USES AUXILIARY SUB-FUNCTIONS

None.

DATA GRANULE

One Scan

5.2.9.1 Objectives

To apply generic South Atlantic Anomaly, Sunglint and Rainbow checks to data from all measurement modes based on geolocation and viewing information calculated in Calculate Geolocation for Fixed Grid (A2.6).

5.2.9.2 Description

Generic SAA, sunglint and rainbow checks are applied to data from all measurement modes on the basis of geolocation and viewing information calculated in Calculate Geolocation for Fixed Grid (A2.6). These checks are applied to all data including those that may later be excluded from the processing on the basis of subsequent quality checking.

The SAA region will be specified as a rectangular region in longitude and latitude. The check will be evaluated on a scan basis only. Calibration mode data measured in the SAA will not be used in calibration processing. Sunglint and Rainbow are phenomena that invalidate the calculation of air mass factors in level 2 processing and must be flagged during Level 0 to 1a Processing (A2). Two thresholds for low and high sunglint danger will be used. Sunglint and rainbow are strongly dependent on the observing geometry. The flag simply indicates a geometrical possibility. The check is evaluated for shortest effective integration time of the main channels (187.5 ms, R_{FPA} = 32 times per scan) independent of the actual integration time.

5.2.9.3 Variables

5.2.9.4 Input/ from Initialisation Dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
$\theta_{termDark}$	Solar zenith angle in the Northern hemisphere which defines the terminator as appropriate for dark signal measurements.	d	degrees	*i*	A2.0.1	
$\Theta_{termEarth}$	Solar zenith angle in the Northern hemisphere which defines the terminator as appropriate for Earth measurements.	d	degrees	*i*	A2.0.1	

5.2.9.4.1 *Input/output from Other Functions*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
mode	Observation mode	enum	degrees	*i*	A2.3	
lon_{Sat}	Geocentric longitude of the satellite and SSP (earth-fixed CS)	d[R_{FPA}]	degrees	*i*	A2.6	Only lon_{Sat}[0] is used.
lat_{Sat}	Geodetic latitude of the satellite and SSP (earth-fixed CS)	d[R_{FPA}]	degrees	*i*	A2.6	Only lon_{Sat}[0] is used.
θ	Line-of-sight zenith angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degrees	*i*	A2.6	
θ_0	Solar zenith angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degrees	*i*	A2.6	
φ	Line-of-sight azimuth angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degrees	*i*	A2.6	
φ_0	Solar azimuth angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degrees	*i*	A2.6	
Θ	Scattering angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degrees	*i*	A2.6	
Θ_{Sun}	Solar zenith (Satellite Relative Actual Reference CS)	d[R_{FPA}]	degrees	*i*	A2.6	

5.2.9.5 Global PCDs Accumulated per Product

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
N_{SAA}	Number of scans in the SAA	w	-	*g*	A2.22	
$N_{sunglint}$	Number of scans with sunglint danger	w	-	*g*	A2.22	
$N_{rainbow}$	Number of scans with rainbow danger	w	-	*g*	A2.22	
$N_{mode,geo}$	Number of scans with possible mismatch between observation mode and geolocation.	w	-	*g*	A2.22	

5.2.9.5.1 *Output*

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
F_{SAA}	Flag indicating scan is in the SAA	bit-string [32]	-	o	A2.23.1	**MDR-1*** PCD_BASIC F_SAA 1 = in SAA 0 = not in SAA
$F_{sunglint}$	Flag indicating risk of sunglint per scan	enum [R_{FPA}]	-	o	A2.23.1	**MDR-1*** PCD_BASIC F_SUNGLINT_RISK
$F_{sunglint\_high\_risk}$	Flag indicating high risk of sunglint per scan	enum [R_{FPA}]	-	o	A2.23.1	**MDR-1*** PCD_BASIC F_SUNGLINT_HIGH_RISK
$F_{rainbow}$	Flag indicating danger of rainbow per scan	bool [R_{FPA}]	-	o	A2.23.1	**MDR-1*** PCD_BASIC F_RAINBOW 1 = risk 0 = no risk
$F_{mode,geo}$	Flag indicating possible mismatch between observation mode and geolocation	bool [R_{FPA}]	-	o	A2.23.1	**MDR-1*** PCD_BASIC F_MODE_GEOLOCATION 1 = mismatch 0 = match

5.2.9.6 Algorithm

- The required geolocation and line of sight angles have been calculated previously in Calculate Geolocation for Fixed Grid (A2.6).
- Generate an SAA flag F_{SAA} using Check for SAA (AG.8) with coordinates $lon_{Sat}[0]$ and $lat_{Sat}[0]$ on input.
  N_{SAA} is assumed to be initialised to zero at the start of processing a product so for all readouts

$N_{SAA} = N_{SAA} + 1$	*Equation 62*

- If mode is one of the six modes in the earth category, generate sunglint flags $F_{sunglint\_risk}$ and $F_{sunglint\_high\_risk}$ using Check for Sunglint (AG.9). $N_{sunglint}$ is assumed to be initialized to zero at the start of processing a product, so for all readouts k if any of $F_{sunglin\_high\_risk.k} = 1$ or $F_{sunlight\_risk.k} = 1$ then:

$N_{sunglint} = N_{sunglint} + 1$	*Equation 63*

- If *mode* is one of the six modes in the earth category, generate a rainbow flags $F_{rainbow}$ using Check for Rainbow (AG.10). $N_{rainbow}$ is assumed to be initialised to zero at the start of processing a product so for all readouts k, if any of $F_{rainbow,k} = 1$.

$N_{rainbow} = N_{rainbow} + 1$	*Equation 64*

- Initialise the flag $F_{mode,geo}$ to zero. Using the observation mode *mode* and the solar zenith angle Θ_{Sun}, set $F_{mode,geo}$ to one if one of the following conditions is fulfilled:
  1. Dark measurements outside eclipse: *mode* = *Dark* and $\min(\Theta_{Sun}) < \Theta_{termDark}$.
  2. Earth measurements within eclipse: *mode* = one of the six modes in the earth category and $\max(\Theta_{Sun}) > \Theta_{termEarth}$.
  3. Solar measurements with the sun far outside the solar field of view: *mode* = *Sun* and $\min(|\Theta_{Sun} - 90|) > 5$.

  Set:

$N_{mode,geo} = N_{mode,geo} + F_{mode,geo}$	*Equation 65*

5.2.10 Calculate Dark Signal Correction (A2.8)

Instrument Modes		***Instrument Data***	
Earth		PMD	√
Dark	√	FPA	√
Sun		Housekeeping	√
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

USES GENERIC SUB-FUNCTIONS

None

USES AUXILIARY SUB-FUNCTIONS

Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1)
Linear Interpolation (AX.2)

DATA GRANULE

All scans from one *dark* calibration mode measurement period.

5.2.10.1 Objectives

To calculate dark signal correction parameters on the basis of all measurements made in dark calibration mode, on the dark side of the orbit.

5.2.10.2 Description

The calculation of the dark signal correction requires all measurements taken during the dark calibration mode, acquired on the dark side of the orbit, to be collected, excluding the measurements for a time period t_{stab}^{Dark} after switching to dark observation mode. The observation mode is determined on a scan basis (Section 5.2.5). All scans for which the observation mode is *dark* are accumulated. Individual readouts are read from each scan. As the measured dark signal is dependent on both integration time, the accumulated scans must be sorted on the basis of integration time. This algorithm describes the calculation for a specific integration time after collection and reading of the scans is done. Data must also be sorted into all combinations of PMD readout and transfer mode as specified in Appendix B.

The dark signal correction is calculated as the mean of all *dark* detector pixel readouts for each band. The readout noise is calculated as the standard deviation of the *dark* detector pixel readouts for each band. The calculations are carried out using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1). The data has previously been checked for saturated pixels and hot pixels using Determine PCDs from Raw Intensity (A2.4).

Note: Dark signal measurements taken in regions with a high background of cosmic rays such as the South Atlantic Anomaly (SAA) as described in Section 5.7.8 shall be excluded from calibration processing.

5.2.10.3 Variables

5.2.10.3.1 Local variables

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
N	Total number of scans to be accumulated and averaged	i	-	t	-	
σ_{dt}	Dark signal detector temperature standard deviation for all dark signal readouts used	d[B]	K	i	-	

5.2.10.3.2 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
$\theta_{DarkCut}$	Solar zenith angle in the Northern hemisphere which defines the terminator as appropriate for cutting off dark signal measurements.	d	degrees	i	A2.0.1	118.0
t_{stab}^{Dark}	Stabilisation time for dark signal measurements	d	*s*	i	A2.0.1	
t_{min}^{Dark}	Minimum duration time for dark signal measurements	d	*s*	i	A2.0.1	
$t_{\overline{DS}}$	Threshold for mean dark signal per band	i[B]	BU	i	A2.0.1	
$t_{\overline{\sigma_D}}$	Threshold for mean dark signal readout noise per band	i[B]	BU	i	A2.0.1	
offset	Dark signal electronic offset	i[B]	BU	i	A2.0.1	
$t_{\sigma_{di}}$	Threshold for dark signal detector temperature standard deviation	d	K	i	A2.0.1	
$discard_{dt}$	Temperature difference below which a previous dark signal correction is discarded from a data set containing only most recent inflight calibration data records	d	K	i	A2.0.1	*Currently* = σ_{dt}

5.2.10.3.3 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
IT	Integration time to be used for sorting of *dark* observation mode scans	d[B,N]	s	i	A2.2	
dt	Detector temperature to be used for calculation of the mean detector temperature of *dark* observation mode scans	d[B	*K*	i	A2.2	
UTC_{dark}	UTC date/time of *Dark* calibration mode measurements	d[B	fractional days	i	A2.3	
pmd_transfer	PMD transfer mode to be used for sorting of *dark* observation mode scans	enum[N]	-	i	A2.3	
pmd_readout	PMD readout mode to be used for sorting of *dark* observation mode scans	enum[N]	-	i	A2.3	
θ_0	Solar zenith angle, *h*0, point F (topocentric CS)	$d[R_{FPA}]$	degrees	i	A2.6	
F_{SAA}	Flag indicating whether scan is in the SAA	bit-string [32,N]	-	i	A2.7	1 = in SAA 0 = not in SAA
missing	Mask indicating missing mean values	bool[D,B]	-	i	AX.1	1 = missing 0 = not missing
S	Dark signal readouts	d[D,B,N]	BU	i	A2.0.7	

5.2.10.3.4 Input from level 0 data stream

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
S	Dark signal readouts	d[D,B,N]	BU	i	A2.0.7	

5.2.10.3.5 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/Remarks*
DS_{start}	Start UTC date/time of valid *Dark* calibration mode measurements	d	fractional days	o	ifc	
DS_{end}	End UTC date/time of valid *Dark* calibration mode measurements	d	fractional days	o	ifc	
DS_{IT}	Integration time for which dark signal correction is valid	d[B]	s	o	ifc	
DS_{dt}	Mean detector temperature for which dark signal correction is valid	d[B]	K	o	ifc	
$DS_{transfer}$	*pmd_transfer* mode for which dark signal correction is valid	enum	-	o	ifc	
$DS_{readout}$	*pmd_readout* mode for which dark signal correction is valid	enum	-	o	ifc	
DS	Dark signal correction	d[D,B]	BU	o	ifc	
σ_D	Standard deviation in dark signal readout values equivalent to readout noise.	d[D,B]	BU	o	ifc	
$\overline{DS}$	Dark signal correction averaged per band.	d[B]	BU	o	ifc	
σ_D	Dark signal correction readout noise averaged per band.	d[B]	BU	o	ifc	
$F_{\overline{DS}}$	Flag indicating whether dark signal correction averaged per band exceeds specified threshold	bool[B]	-	o	ifc	
$F_{\overline{\sigma_D}}$	Flag indicating whether dark signal correction readout noise averaged per band exceeds specified threshold	bool[B]	-	o	ifc	
F_D^{miss}	Flag indicating that missing mean *Dark* calibration mode measurements have been filled by interpolation or that one complete band is missing	enum[B]	-	o	ifc	

5.2.10.4 Algorithm

5.2.10.4.1 Sort Scans From Dark Observation Mode (A2.8.1)

All scans in one *dark* observation mode period, excluding the measurements for a time period t_{stab}^{Dark} after switching to *dark* observation mode and excluding readouts for which $\theta_0 < \theta_{DarkCut}$, are accumulated. If scans have been accumulated for a duration less than t_{min}^{Dark} the data are discarded. Otherwise, accumulated scans are sorted on the basis of integration time *(IT)*, PMD transfer mode *(pmd_transfer)* and PMD readout mode *(pmd_readout)*. The following calculation of dark signal correction applies to each sorted group. Main channel bands should be separated for the calculation of dark signal correction. Also, in the case of signals co-added on-board the *actual* integration time–not the *effective* integration time after co-adding–is used.

5.2.10.4.2 Calculate Mean and Standard Deviation Of All Dark Readouts (A2.8.2)

Calculate the mean and standard deviation for each detector pixel of each band from all dark signal readouts, *N*, collected during one *Dark* calibration period using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1). Scans for which $F_{SAA} = 1$ for any readout are excluded from the calculation of dark signal correction.

5.2.10.4.3 Calculate Dark Signal Correction and Readout Noise (A2.8.3)

The dark signal correction *DS* is equal to the mean dark signal readout for each detector pixel of each band. The readout noise σ_D is equal to the standard deviation of the dark signal readouts from each band. Any detector pixels for which there are no valid readouts, as indicated by *missing*, are assigned mean values which are equal to a linear interpolation between the nearest valid neighbouring values calculated using Linear Interpolation (AX.2). In the case that an entire band is missing, no dark signal correction is calculated for that band. For FPA records set $DS_{transfer}$ and $DS_{readout}$ to various. For PMD records, including short wavelength bands, set them to the actual PMD transfer and readout modes. The dark signal detector temperature DS_{dt} is calculated as the mean of the detector temperature *dt* for all dark signal readouts used. If σ_{dt} of all dark signal measurements used is above the threshold $t_{\sigma_{dt}}$, the dark signal correction is discarded.
Before adding a newly created dark signal correction to a data set containing only the most recent in-flight calibration data, old dark signal corrections with a mean temperature DS_{dt} within $discard_{dt}$ of the new record shall be discarded from this data set although all in-flight calibration data shall be stored for monitoring purposes for the lifetime of the mission.

5.2.10.4.4 Calculate PCDs For Dark Signal Correction (A2.8.4)

For *j* = 1...*B* then

$$\overline{DS_j} = \sum_{i=0}^{D_j-1} \frac{DS_{ij}}{D_j} \text{ and } \overline{\sigma_{D,j}} = \sum_{i=0}^{D_j-1} \frac{\sigma_{D,ij}}{D_j}$$

Equation 66

Note: In Equation 66, only spectral averaging is applied. Averaging over readouts has already been performed in steps A2.8.2 and A2.8.3.

Assuming $F_{\overline{DS}}$ and $F_{\overline{\sigma_D}}$ have been initialised to zero then if

$$(\overline{DS}_j - offset_j)/IT_j > t_{\overline{DS},\, j} \text{ then } F_{\overline{DS},\, j} = 1 \quad \text{Equation 67}$$

and if

$$\overline{\sigma_{D,\, j}} > t_{\overline{\sigma_D},\, j} \text{ then } F_{\overline{\sigma_D},\, j} = 1 \quad \text{Equation 68}$$

Set $F_{D,j}^{miss}$ to:

- *some_missing* if interpolated values were included in the dark signal correction for band *j* as a result of missing mean values,
- *all_missing* if the entire band *j* is missing,
- *no_missing* otherwise.

5.2.11 APPLY DARK SIGNAL CORRECTION (A2.9)

Instrument Modes		***Instrument Data***	
Earth (PMD only)	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser			
LED	√		
Moon			
Other			

USES GENERIC SUB-FUNCTIONS

Apply Dark Signal Correction (AG.11)

USES AUXILIARY SUB-FUNCTIONS

None

DATA GRANULE

One Scan

5.2.12 NORMALISE SIGNALS TO ONE SECOND INTEGRATION TIME (A2.10)

Instrument Modes		*Instrument Data*	
Earth (PMD only)	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon			
Other			

USES GENERIC SUB-FUNCTIONS

Normalise signals to one second integration time (AG.12)

USES AUXILIARY SUB-FUNCTIONS

None

DATA GRANULE

One Scan

5.2.13 CALCULATE PPG (A2.11)

Instrument Modes		*Instrument Data*	
Earth (PMD only)		PMD	√
Dark		FPA	√
Sun		Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED	√		
Moon			
Other			

USES GENERIC SUB-FUNCTIONS

None

USES AUXILIARY SUB-FUNCTIONS

Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1)
Linear Interpolation (AX.2)

DATA GRANULE

All scans from one *LED* calibration mode measurement period.

5.2.13.1 Objectives

To determine the Pixel to Pixel Gain (PPG) correction using measurements taken in *LED* calibration mode (Section 2.3.3).

5.2.13.2 Description

Adjacent pixels on an array detector may have slightly different Quantum Efficiency, otherwise known as Pixel-to-Pixel Gain (PPG). This PPG pattern is superimposed on all other calibration and earthshine measurements. It is necessary to remove the PPG gain before proceeding further with the processing of calibration measurements. PPG is determined using measurements taken in *LED* calibration mode (Section 5.2.5) anticipated to be part of the monthly calibration timeline. When GOME-2 is in *LED* calibration mode the detector arrays are illuminated with light from onboard LEDs without spectral dispersion. Deviations from spectrally smooth behaviour in the measurements may be attributed to PPG.

The calculation of PPG from LED measurements requires that all scans from one *LED* mode calibration period are collected. PMD data are assumed to be transferred in raw transfer mode. If this is not the case PMD data are excluded from the calculations. Individual readouts are read from each scan. LED readouts are first corrected for dark signal and normalised to one-second integration time. Then, to maximise signal to noise in the measurements, a mean LED spectrum is calculated for each channel from all readouts, excluding the measurements for a time period t_{stab}^{LED} after LED switch-on as determined from the LED status bits. The calculations are carried out using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1). The data has previously been checked for saturated pixels and hot pixels using Determine PCDs from Raw Intensity (A2.4). Each mean LED spectrum is then smoothed using a triangular or a polynomial smoothing function of width $2 \times sm_{LED} + 1$. The finite number of end detector pixels of a channel which are not smoothed have a PPG of one assigned. Note that *LED* calibration-mode measurements taken in the South Atlantic Anomaly (SAA) as described in Section 5.7.8shall be excluded from calibration processing.

The PPG gain correction for each detector pixel is calculated as the ratio of the mean to the smoothed LED measurement.

5.2.13.3 Variables

5.2.13.3.1 Local variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
k	Detector pixel index counter	i	-	t	-	
N	Total number of scans to be accumulated and averaged.	i	-	t	-	
$\overline{S_{LED}}^{sm}$	Smoothed mean LED spectrum	d[D,B]	BU/s	t	-	

5.2.13.3.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
PPG_back	Switch for selection of backup source (WLS) in event of LED failure	enum	-	i/o	A2.0.1/ife	
t_{stab}^{LED}	Stabilisation time for LEDs	d	s	i	A2.0.1	
$t_{\overline{PPG}}$	Threshold for PPG correction averaged per channel	d[B]	-	i	A2.0.1	
$t_{\sigma PPG}$	Threshold for standard deviation in PPG per channel	d[B]	-	i	A2.0.1	
smLEDtype	Switch for selection of smoothing function	enum	-	i	A2.0.1	0 = triangular 1 = polynomial
sm_{LED}	Smoothing width	i	pixel	i	A2.0.1	

5.2.13.3.3 Input/output from other functions

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
UTC_{LED}	UTC date/time of *LED* calibration mode readouts	d[N]	fractional days	i	A2.3	
pmd_transfer	PMD transfer mode	enum[N]	-	i	A2.3	
F_{SAA}	Flag indicating whether scan is in the SAA	bit-string [32,N]	-	i	A2.7	1 = in SAA 0 = not in SAA

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
HK	Housekeeping data	w[488]	-	i	A2.0.7	Only ICU word 2 (containing LED status) is used, see [AD 9]
S_{LED}	Detector readout values from *LED* calibration mode, corrected for dark signal and normalised to one-second integration time.	d[D,B,N]	BU/s	i	A2.10	
$\overline{S_{LED}}$	Mean LED detector readouts	d[D,B]	BU/s	i	AX.1	
missing	Mask indicating missing mean values	i[D,B]	-	i	AX.1	1 = missing 0 = not missing

5.2.13.3.4 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
LED_{start}	Start UTC date/time of valid *LED* (or *WLS*) calibration mode measurements	d	fractional days	o	ifc	
LED_{end}	End UTC date/time of valid *LED* (or *WLS*) calibration mode measurements	d	-	o	ifc	
PPG	Pixel to Pixel Gain correction	d[D,B]	-	o	ifc	
$\overline{PPG}$	Mean PPG correction per channel	d[B]	-	o	ifc	
$F_{\overline{PPG}}$	Flag indicating whether PPG averaged per channel exceeds specified threshold	bool[B]	-	o	ifc	
$F_{\sigma PPG}$	Flag indicating whether standard deviation of PPG per channel exceeds specified threshold	bool[B]	-	o	ifc	1 = exceeds 0 = does not
F_{PPG}^{miss}	Flag indicating that missing mean *LED* calibration mode measurements have been filled by interpolation or that one complete channel is missing	enum[B]	--	o	ifc	
F_{PPG}^{LED}	LED status flag	b	-	o	ifc	See [AD 9]

5.2.13.4 Algorithm

If *pmd_transfer* = *raw* (i.e. PMD data is transferred in raw mode) the following calculations are carried out for both main and PMD channels. Otherwise the calculations are carried out for main channels only. Nothing is done for PMD channels. Note also that PPG correction is calculated per channel. Main channel bands need only be separated for the calculation of a mean LED readout. LEDs can be switched on separately for the main channels (chain 1) and the PMD channels (chain 2). The PPG correction is calculated only for those channels where the LEDs are switched on.

5.2.13.4.1 Calculate Mean of All LED Readouts (A2.11.1)

The mean LED, dark signal corrected detector readout normalised to one-second integration time, and the noise in the mean are calculated using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1), excluding the measurements for a time period T_{stab}^{LED} after LED switch-on as determined from the LED status bits. Scans for which F_{SAA} = 1 for any readout are excluded from the calculation of PPG correction. Any detector pixels for which there are no valid readouts, as indicated by *missing*, are assigned mean values which are equal to a linear interpolation between the nearest valid neighbouring values calculated using Linear Interpolation (AX.2). In the case that an entire channel is missing, no PPG correction is calculated for that channel.

5.2.13.4.2 Calculate PPG (A2.11.2)

If *smLEDType* = 0 then the mean LED spectrum is then smoothed using a triangular smoothing function of width 2 × sm_{LED} + 1 such that for $i = sm_{LED}...D_j - sm_{LED}$ and $j = 1...B$:

$$\bar{S}_{ij}^{sm} = \frac{1}{(sm_{LED})^2} \cdot \left(\sum_{k=-sm_{LED}}^{sm_{LED}} (sm_{LED} - |k|) \cdot \bar{S}_{(i+k),j} \right)$$

Equation 69

If *smLEDType* = 1 then the mean LED spectrum is smoothed by fitting a third order polynomial smoothing function of width 2 × sm_{LED} + 1 centered on pixel *i* for $i = sm_{LED}...D_j - sm_{LED}$ and $j = 1...B$:

The smoothed spectrum $\bar{S}_{ij}^{sm}$ is then calculated for pixel *i* and channel *j* as the mean of the fitted polynomial.

The PPG is then calculated for $i = sm_{LED}...D_j - sm_{LED}$ and $j = 1...B$ as the following:

$$PPG_{ij} = \frac{\bar{S}_{ij}}{\bar{S}_{ij}^{sm}}$$

Equation 70

For $i = 0...sm_{LED} - 1$, $i = D_j - sm_{LED}...Dj - 1$ and $j = 1...B$

$$\bar{S}_{ij}^{sm} = \bar{S}_{ij} \text{ and } PPG_{ij} = 1.0$$ *Equation 71*

5.2.13.4.3 Calculate PCDs from PPG Correction (A2.11.3)

The lower (least significant) 4 bits of the LED status flag F_{PPG}^{LED} are set to be the same as the four bits of the LED status in the ICU word 2 of the housekeeping data *HK*. The upper four bits F_{PPG}^{LED} are set to zero.

For $j = 1...B$, then

$$\overline{PPG}_j = \sum_{i=0}^{D_j-1} \frac{PPG_{ij}}{D_j} \text{ and } \sigma_{PPG,j} = \sqrt{\frac{1}{D_j - 1} \cdot \sum_{i=0}^{D_j-1} (PPG_{ij} - \overline{PPG}_j)^2}$$ *Equation 72*

Assuming $F_{\overline{PPG}}$ and $F_{\sigma_{PPG}}$ have been initialised to zero then if:

$$\left|\overline{PPG}_j - 1\right| > t_{\overline{PPG},j} \text{ then } F_{\overline{PPG},j} = 1$$ *Equation 73*

and if

$$\sigma_{PPG,j} > t_{\sigma_{PPG},j} \text{ then } F_{\sigma_{PPG},j} = 1$$ *Equation 74*

Set $F_{PPG,j}^{miss}$ to

- *some_missing* if interpolated values were included in the mean signals for band *j* as a result of missing mean values,
- *all_missing* if the entire band *j* is missing,
- *no_missing* otherwise.

5.2.13.4.4 Backup Algorithm: Calculate PPG Correction from WLS Measurements (A2.11.4)

If *PPG_backup* = *WLS* then calculate the PPG correction using the WLS spectrum. The specific algorithm to be used is as described above with the exception that *LED* is replaced by *WLS*.

5.2.14 APPLY PPG CORRECTION (A2.12)

Instrument Modes		*Instrument Data*	
Earth (PMD only)		PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS	√		
SLS	√		
SLS over Diffuser			
LED			
Moon			

USES GENERIC SUB-FUNCTIONS

Apply PPG Correction (AG.13)

USES AUXILIARY SUB-FUNCTIONS

None

DATA GRANULE

One Scan.

5.2.15 CALCULATE SPECTRAL CALIBRATION PARAMETERS FOR MAIN CHANNELS (A2.13)

Instrument Modes		*Instrument Data*	
Earth (PMD only)		PMD	
Dark		FPA	√
Sun		Housekeeping	
WLS			
SLS	√		
SLS over Diffuser			
LED			
Moon			
Other			

USES GENERIC SUB-FUNCTIONS

None

USES AUXILIARY SUB-FUNCTIONS

Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1)

DATA GRANULE

All scans from one SLS calibration mode period.

5.2.15.1 Objectives

Calculate spectral calibration coefficients for main channels from preprocessed SLS spectra.

5.2.15.2 Description

GOME-2 spectra are acquired by linear diode array detectors. The spectrum is dispersed across the diode array, so that each detector pixel (centre) corresponds to a particular wavelength. Spectral calibration is the assignment of a wavelength value to each detector pixel. For each GOME-2-channel, a low order polynomial approximation will be used to describe wavelength as a function of detector pixel. This module derives the polynomial coefficients for the main channels from pre-processed spectra of the Spectral Light Source (SLS) which provides a number of narrow spectral lines at known wavelengths across the GOME-2 wavelength range. The module Apply Spectral Calibration (AG.14) will calculate the wavelength for each detector pixel from these polynomial coefficients later in the process.

The GOME-2 SLS is a gas discharge lamp with a Platinum/Chromium hollow cathode and a mixture of 90% Neon and 10% Argon as a fill gas. Emission lines of the cathode material dominate in main channel 1 while mainly Neon and Argon lines contribute to the emission in channels 2 to 4. The actual width of the individual emission lines (dominated by the Doppler width) is much smaller than the spectral resolution of GOME-2 and will be neglected in the following. In order to be usable for main channel wavelength calibration, a line is required to be sufficiently separated from neighbouring lines, and to have sufficient intensity. Furthermore, the number of selected lines per channel must not be smaller than the number of polynomial coefficients to be deter-mined, and the lines should be well distributed across the channel. The list of selected usable lines represents a compromise between these requirements. It will be specified in the initialisation data-set, making use of recommendations from pre-flight characterisation and calibration.

This module expects a series of dark signal and PPG-corrected SLS main channel measurements, normalised to one-second integration time, on input. First, the relevant measurements are aver-aged, skipping the first measurements after lamp switch-on to allow stabilisation of the lamp out-put. From the averaged SLS spectrum, the spectral calibration coefficients for the main channels are derived and checked in four steps:

1. A line-finding algorithm identifies the selected spectral lines. A first quality check is per-formed in order to exclude lines not fulfilling required criteria, e.g., lines for which the signal level is too low.
2. The fractional pixel positions and some further statistical diagnostics (FWHM, skew) for each of the remaining spectral lines are calculated. A second quality check using these results is performed and lines outside the required criteria on FWHM and skew are excluded. Option-ally, fractional pixel positions are corrected for biases using a mapping term from the instrument calibration key data.
3. A low-order polynomial is fitted to the set of remaining spectral lines.
4. As a quality check, the actual line positions (from step 2) are compared to the positions calculated from the polynomial.

Note: For the PMD channels, a different algorithm has to be applied as their lower spectral resolution does not allow the separation of individual emission lines (see Section 1).

5.2.15.3 Variables

5.2.15.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
k	Spectral line index	*i*		*t*		*1…K*
m	Polynomial coefficient index	*i*		*t*		*0…M*
n	Range index	*i*		*t*		*0…1*

5.2.15.3.2 Local variables

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
N	Total number of scans to be accumulated and averaged.	i	-	t	-	
σ_{pdpt}	Pre-disperser prism temperature standard deviation for all read-outs used	d[B]	K	t	-	
i_s	Pixel range (start/end pixel) for search window	i[2]	pix	t	-	
$\overline{S}_{max}$	Maximum averaged signal within search window	d	BU/s	t	-	
i_{max}	Pixel position of maximum signal within search window	i	pix	t	-	
i	Pixel range (start/end pixel) for statistics window, including one pixel on either side for back-ground subtraction	i[2]	pix	t	-	
$\hat{S}$	Signal per detector pixel in statistics window after background subtraction	d[w]	BU/s	t	-	
S_{tot}	Total signal in statistics window after background subtraction	d	BU/s	t	-	
COG	Centre of gravity per line and channel	d[K_{cha}, B_{FPA}]	pix	t	-	
σ	Variance per line and channel	d[K_{cha}, B_{FPA}]	pix^2	t	-	
$Skew$	Skewness per line and channel	d[K_{cha}, B_{FPA}]	pix^3	t	-	
$FWHM$	Full width at half maximum perline and channel	d[K_{cha}, B_{FPA}]	pix	t	-	

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
K	Number of lines remaining per channel after all selection criteria have been applied	$i[B_{FPA}]$	-			
x	Retrieved position of SLS line per main channel, given as fractional pixel number normalised to the interval [0…1]	$d[K, B_{FPA}]$	-			

5.2.15.3.3 *Input from initialisation dataset*

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
t_{stab}^{SLS}	Stabilisation time for SLS lamp	d	s	i	A2.0.1	
U_{on}^{SLS}	SLS lamp voltage used to deter-mine whether lamp is on	d	V	i/o	A2.0.1	
U_{lvm}^{SLS}	SLS lamp voltage for low volt-age mode	d	V	i/o	A2.0.1	
δ_{pdp}	Pre-disperser prism temperature tolerance	d	K	i	A2.0.1	
$t_{\sigma_{pdp}}$	Threshold for the pre-disperser prism temperature standard deviation	d	K	i	A2.0.1	
$discard_{pdp}$	Temperature difference below which previous spectral calibration parameters are discarded from a data set containing only most recent in-flight calibration data records	d	K	i	A2.0.1	*currently* $= \sigma_{pdpt}$
M	Order of wavelength calibration polynomial per channel	i[B]	-	i	A2.0.1	
Δ	Search window used for line-finding around first-guess pixel position per channel	$i\ [B_{FPA},2]$	pix	i	A2.0.1	
S_{req}	Minimum required peak signal for a line to be accepted	i	BU	i	A2.0.1	
w	Width of statistics window around a line, per channel	$i[B_{FPA}]$	pix	i	A2.0.1	
$FWHM_{max}$	Maximum full width at half maximum for line to be accepted per channel	$d[B_{FPA}]$	pix	i	A2.0.1	
$Skew_{max}$	Maximum skewness for a line to be accepted per channel	$d[B_{FPA}]$	pix^3	i	A2.0.1	
$t_{\delta_{max}}$	Threshold for maximum deviation between fitted line positions and true line positions.	$d[B_{FPA}]$	mn	i	A2.0.1	

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
MapSLS	Flag indicating whether to apply the mapping to external SLS in the main channel spectral calibration	bool	-	i	A2.0.1	0 = do not perform mapping 1 = perform mapping (default)

5.2.15.3.4 Input from key dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
K_{tot}	Number of used SLS lines	i	-	i	A2.0.4	
λ	Position of SLS line given as vacuum wavelength	$d[K_{tot}]$	nm	i	A2.0.4	This is channel independent
i_0	Position of SLS lines given as fractional pixel number per main channel (for the instrument in vacuum)	$d[K_{tot}, B_{FPA}]$	pix	i	A2.0.4	To be used as first-guess position for line finding
$\delta\lambda$	Mapping of SLS line position between external and internal SLS (external – internal).	$d[K_{tot}, B_{FPA}]$	pix	i	A2.0.4	This is channel dependent! External SLS line positions (during on-ground calibration) are considered more reliable, so this is a correction term for the internal SLS line positions which might have a bias.

5.2.15.3.5 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
pdp	Pre-disperser prism temperature used for calculation of the mean pre-disperser prism temperature of SLS observation mode scans	d[n]	K	i	A2.2	*expected to be stable over one SLS calibration mode period*
U^{SLS}	SLS lamp voltage	d	V	i	A2.2	
IT	Integration time per band	i[B,N]	s	i	A2.2	

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
UTC_{SLS}	UTC date/time of SLS calibration mode measurements	d[N]	fractional days	i	A2.3	
F_{SAA}	Flag indicating whether scan is in the SAA	bit-string[32,N]	-	i	A2.3	1 = in SAA 0 = not in SAA
S	SLS main channel signals, dark signal and PPG corrected, and normalised to one-second integration time	d[D,B_{FPA}, N]	BU/s	i	A2.12	
missing	Mask indicating missing mean values	i[D,B]	-	i	AX.1	1 = missing 0 = not missing

5.2.15.3.6 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
SLS_{start}	Start UTC date/time of valid SLS calibration mode measurements	d	fractional days	o	ifc	
SLS_{end}	End UTC date/time of valid SLS calibration mode measurements	d	fractional days	o	ifc	
SLS_{pdp}	Mean pre-disperser prism tem-premature for which spectral calibration is valid	d	K	o	ifc	
$\overline{S}^{FPA}$	Averaged SLS main channel signals	d[D,B_{FPA}]	BU/s	o	A2.15	
a	Polynomial coefficients	d[B,max(M)]	nm	o	ifc	See (Equation 75).
N_{lines}	Number of lines accepted for use in spectral calibration per channel.	w[B_{FPA}]	–	o	ifc	
δ_{max}	Maximum deviation between fitted and true line position per channel	d[B_{FPA}]	nm	o	ifc	
$\overline{\delta}$	Average deviation between fitted and true line position per channel	d[B_{FPA}]	nm	o	ifc	

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
δ	Deviation between fitted line position and true line positions.	$d[N_{lines},B_{FPA}]$	nm	o	ifc	
F_{lines}	Flag indicating whether number of lamp lines accepted for use in spectral calibration is below order of wavelength calibration polynomial M per channel	$bool[B_{FPA}]$	-	o	ifc	1 = number of lines too low 0 = number of lines sufficient
$F_{\delta_{max}}$	Flag indicating whether maximum deviation between fitted line positions and true line positions exceeds specified threshold.	$bool[B_{FPA}]$	-	o	ifc	1 = exceeds 0 = does not
F^{miss}_{SLS}	Flag indicating that no spectral calibration was generated due to missing mean SLS mode measurements per channel	bool[B]	-	i/o	ifc	

5.2.15.4 Algorithm

Note that spectral calibration is calculated per channel. Main channel bands need only be separated for the calculation of a mean SLS readout. Main channel bands need only be separated for the calculation of a mean SLS readout.

5.2.15.4.1 Average Relevant SLS Measurements (A2.13.1)

Average FPA spectra *S* from one SLS calibration sequence using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1), excluding the measurements for a time period t_{stab}^{SLS} after lamp ignition as determined from the SLS current (ignition being reached when the SLS current exceeds I_{low}^{SLS} for the first time). This gives an averaged FPA spectrum $\overline{S^{FPA}}$. Main channel bands need only be separated for the calculation of a mean SLS readout. Scans for which $F_{SAA} = 1$ for any readout are excluded from the calculation of spectral calibration coefficients. In the case that there are detector pixels with no valid readouts in any channel as indicated by *missing*, no spectral calibration coefficients are generated for that channel.

5.2.15.4.2 Calculate Spectral Calibration Parameters (A2.13.2)

Polynomial coefficients a_{jm} will be derived from the line positions of the SLS such that for detector pixel number *i* in main channel *j*, the wavelength λ_{ij} of the pixel centre can be expressed as the following:

$$\lambda_{ij} = \sum_{m=0}^{M_j} a_{jm} (i/1023.0)^m \qquad \textit{Equation 75}$$

The normalisation of the detector pixel numbers from the interval [0…1023] to the interval [0…1] is performed in order to avoid numerical under-/overflow in the fitting routines, and to limit the variation of a_{jm} with polynomial index *m*.

The calculation is performed on the averaged SLS measurements $\overline{S^{FPA}}$ from the previous step.

Checks for detector pixel numbers to be in the valid range (0…1023) are not mentioned explicitly. They have to be performed as needed.

Loop information: The following calculations are performed for each of the four main channels.

5.2.15.4.2.1 Find Spectral Lines

If $U^{SLS} < U_{lam}^{SLS}$ use specific spectral line key data (WL_LINEPOS_MAIN_LOW) instead of the standard one (WL_LINEPOS_MAIN). For each of the spectral lines *k* falling within the current channel *j*, determine the maximum signal $\overline{S}_{max}$ within the pixel range $[i_{S0} \ldots i_{S1}]$ (the "search window") and its pixel position i_{max}, where i_{S0} = Round($i_{kj,0}$)+Δ_{j1} and i_{S1} = Round($i_{kj,0}$) + Δ_{j2}. Note that $\Delta_{j1} < 0$. The search window is not necessarily symmetrical around the first-guess line position $i_{kj,0}$. Accept the line for further processing if the following conditions are fulfilled:

The maximum does not fall on one of the edges of the search window: $i_{S0} < i_{max} < i_{S1}$	*Equation 76*

The required minimum signal is reached: $\bar{S}_{max} \times IT_j > S_{req}$	*Equation 77*

5.2.15.4.2.2 Calculate Statistical Moments for Each Line

For each of the remaining spectral lines k falling within the current channel j, define the pixel range $[i_0 \ldots i_1]$ (the "statistics window") around the maximum i_{max}, where:
$i_0 = i_{max} - (w_j - 1)/2$ and $i_1 = i_{max} + (w_j - 1)/2$.

The statistics window is symmetrical around the line maximum. Subtract a linear baseline correction through the signal values at i_0 and i_1 from the signal:

$$\hat{S}_i = \overline{S^{FPA}}_i - \overline{S^{FPA}}_{i_0} - (\overline{S^{FPA}}_{i_1} - \overline{S^{FPA}}_{i_0})(i - i_0)/(i_1 - i_0),\ i = i_0 \ldots i_1 \qquad \text{Equation 78}$$

Verify that:

$$\hat{S}_i \geq 0 \text{ for all } i = i_0 + 1 \ldots i_1 - 1 \qquad \text{Equation 79}$$

If this is not the case, exclude the line from further processing and continue with the next line. Otherwise, calculate the total signal within the statistics window:

$$\hat{S}_{tot} = \sum_{i = i_0 + 1}^{i_1 - 1} \hat{S}_i \qquad \text{Equation 80}$$

Calculate the first three statistical moments within the statistics window: the centre of gravity.

$$COG_{kj} = \frac{1}{\hat{S}_{tot}} \sum_{i = i_0 + 1}^{i_1 - 1} i\hat{S}_i \qquad \text{Equation 81}$$

the variance

$$\sigma_{kj}^2 = \frac{1}{\hat{S}_{tot} - 1} \sum_{i = i_0 + 1}^{i_1 - 1} (i - COG_{kj})^2 \hat{S}_i \qquad \text{Equation 82}$$

Note: $\sigma_{kj}^2 > 0$ is guaranteed by Equation 81 and the skewness:

$$\text{Skew}_{kj} = \frac{1}{\hat{S}_{\text{tot}}} \sum_{i = i_0 + 1}^{i_1 - 1} \left(\frac{i - \text{COG}_{kj}}{\sigma_{kj}}\right)^3 \hat{S}_i \quad \text{(Equation 83)}$$

The sums in Equation 80 to Equation 83 are carried out from $i_0 + 1$ to $i_1 - 1$ because $\hat{S}_{i0} = \hat{S}_{i1} = 0$ by definition in equation (78). Calculate the full width at half maximum from this:

$$\text{FWHM}_{kj} = \sqrt{8 \ln 2}\, \sigma_{kj} \quad \text{(Equation 84)}$$

Accept the line for further processing if full width at half maximum and skewness do not exceed the allowed values for the current channel:

$$\text{FWHM}_{kj} < \text{FWHM}_{j,\max} \quad \text{(Equation 85)}$$

$$\text{Skew}_{kj} < \text{Skew}_{j,\max} \quad \text{(Equation 86)}$$

After all lines for channel j have been processed, we have K_j lines fulfilling all criteria. For the following, it is assumed that they are (re)numbered from 0 to $K_j - 1$.

5.2.15.4.2.3 Fit Polynomial Through Line Positions

Verify that the remaining number of lines is not smaller than the number of polynomial coefficients to determine for this channel:

$$K_j \geq M_j + 1 \quad \text{(Equation 87)}$$

If this condition is not satisfied, generation of spectral calibration parameters is not done. PCD records as described below shall be generated accordingly.

Normalise the pixel positions to the interval [0...1] for the *Kj* remaining lines, applying the mapping to external SLS line positions as indicated by the *MapSLS* initialisation parameter. Purpose of the mapping is to correct for biases in the line position (in pixels) of the internal SLS, e.g., due to non-homogeneous illumination of the entrance slit.

If no mapping is required (*MapSLS* = 0):

$$x_{kj} = \mathrm{COG}_{kj}/1023,\ k = 0 \ldots K_j - 1$$ *Equation 88*

If mapping is required (*MapSLS* = 1):

$$x_{kj} = (\mathrm{COG}_{kj} + \delta\lambda_{kj})/1023,\ k = 0 \ldots K_j - 1$$ *Equation 89*

Perform SVD fit, as described on page 670 in [RD 10], for the polynomial coefficients a_{jm}, using x_{kj} ($k = 0 \ldots K_j - 1$) as x vector on input, λ_k ($k = 0 \ldots K_j - 1$) as y vector on input, and

$$y = \sum_{m=0}^{M_j} a_{jm} x^m$$ *Equation 90*

as target function.

The pre-disperser prism temperature SLS_{pdp} is calculated as the mean of the pre-disperser prism temperature *pdp* for all SLS readouts used. Note that if σ_{pdpt} for all SLS readouts used is above the threshold $t_{\sigma pdp}$, the spectral calibration parameters are discarded. Before adding newly-created spectral calibration parameters to a data set containing only the most recent in-flight calibration data, old spectral calibration parameters with a mean temperature SLS_{pdp} within $discard_{pdp}$ of the new record shall be discarded from this data set although all in-flight calibration data shall be stored for monitoring purposes for the lifetime of the mission.

5.2.15.4.3 Determine PCDs from Main Channel Spectral Calibration (A2.13.3)

For $j = 1 \ldots B_{FPA}$

$$N_{lines,\,j} = K_j$$ *Equation 91*

and assuming F_{lines} has been initialised to 0, then if:

$$N_{lines,\,j} < M_j + 1 \text{ then } F_{lines,\,j} = 1$$ *Equation 92*

If $F_{lines,\,j} = 0$ calculate the deviations between the fitted line positions and the true line positions:

$$\delta_{kj} = \sum_{m=0}^{M_j} a_{jm} x_{kj}^m - \lambda_k,\ k = 0 \ldots K_j - 1$$ *Equation 93*

and the maximum and mean of the absolute values of δ_{kj} per channel, $\delta_{max,j}$ and $\bar{\bar{\delta}}_j$.

Then, assuming $F_{\delta max}$ has been initialised to 0, then if

$$\delta_{max,\,j} > t_{\delta_{max},\,j} \text{ then } F_{\delta_{max},\,j} = 1$$ *Equation 94*

Set $F^{miss}_{SLS,j}$ to:

- *true* if there are missing mean values in channel *j* and therefore no spectral calibration for this channel,
- *false* otherwise.

5.2.16 CALCULATE SPECTRAL CALIBRATION PARAMETERS FOR PMD CHANNELS (A2.14)

Instrument Modes		Instrument Data	
Earth		PMD	√
Dark		FPA	√
Sun		Housekeeping	
WLS			
SLS	√		
SLS over Diffuser			
LED			
Moon			
Other			

USES GENERIC SUB-FUNCTIONS

Apply Spectral Calibration (AG.14)

USES AUXILIARY SUB-FUNCTIONS

Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1)

DATA GRANULE

Sequence of scans in *SLS* calibration mode.

5.2.16.1 Objectives

Calculate spectral calibration coefficients for PMD channels from preprocessed SLS spectra. Description.

5.2.16.2 Description

This module derives the full spectral grid describing the spectral dispersion of the PMD channels from preprocessed spectra of the Spectral Light Source (SLS). The module Apply Spectral Calibration (AG.14) will later on provide this grid for each detector pixel. See Section 5.2.15 for a general introduction to wavelength calibration of GOME-2 spectra. The algorithm used for the PMD channels is different from the one used for the main FPA channels, because at the lower spectral resolution of the PMD channels individual spectral lines of the SLS cannot be resolved. Instead, an expected PMD spectrum is calculated from the main FPA signals. The spectral shift between the expected and the measured PMD spectrum is then determined by cross-correlating the two in a number of predefined spectral windows.

This module expects a series of dark signal and PPG-corrected SLS PMD measurements and an averaged SLS FPA spectrum on input, both normalised to one-second integration time. First, the relevant PMD measurements are averaged, skipping the first measurements after lamp switch-on to allow stabilisation of the lamp output. Then, the signal expected in the PMD channels for a certain PMD wavelength grid is derived from the measured main channel signal, using the main channel spectral calibration parameters derived in module Calculate Spectral Calibration Parameters for Main Channels (A2.13), Müller matrix elements for PMD and main channels, and the PMD slit function. For a number of spectral windows, the spectral shift between the expected and the measured PMD spectrum is determined by iteratively determining their cross-correlation and updating the expected spectrum with the shift derived from the cross-correlation until convergence is achieved.

PMD data are assumed to be transferred in raw transfer mode and calibration readout mode as described in Appendix B). If this is not the case, nothing is done.

5.2.16.3 Variables

5.2.16.3.1 Indices

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/Remarks*
k	Spectral point (various grids): equidistant wavelength grid SLS Stokes fraction grid	i	-	t	-	$0 \ldots N_E - 1$ $0 \ldots N_q - 1$
m	Polynomial coefficient index	i	-	t	-	$0 \ldots M$
n	PMD index	i	-	t	-	5…6
w	Spectral window index	i	-	t		$0 \ldots N_w - 1$

5.2.16.3.2 Local Variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
N	Total number of scans to be accumulated and averaged.	i	-	t	-	
M^1_Ψ	Radiance response Müller matrix element, interpolated to equivalent SLS viewing angle	d[D,B]	BU.s^{-1} /(photons/(s.cm^2.sr.nm))	t	-	
μ^2_Ψ	Polarisation sensitivity MME ratio M2/M1, interpolated to equivalent SLS viewing angle	d[D,B]	-	t	-	
M^1_Ψ, FPA	Radiance response Müller matrix element, interpolated to equivalent SLS viewing angle and SLS FPA wavelength grid, FPA only	d[D,B_{FPA}]	BU.s^{-1} /(photons/(s.cm^2.sr.nm))	t	-	
μ^2_Ψ, FPA	Polarisation sensitivity MME ratio M^2/M^1, interpolated to equivalent SLS viewing angle and SLS FPA wavelength grid, FPA only	d[D,B_{FPA}]	-	t	-	
M^1_Ψ,PMD	Radiance response Müller matrix element, interpolated to equivalent SLS viewing angle and SLS FPA wavelength grid, PMD only.	d[D,B_{FPA},B_{PMD}]	BU.s^{-1} /(photons/(s.cm^2.sr.nm))	t	-	

Symbol	***Descriptive Name***	***Type***	***Units***	***I/O***	***Source/ Destination***	***References/ Remarks***
μ^2_Ψ, PMD	Polarisation sensitivity MME ratio M^2/M^1, interpolated to equivalent SLS viewing angle and SLS FPA wavelength grid, PMD only	$d[D, B_{FPA}, B_{PMD}]$	-	t	-	
$\bar{S}$	Averaged SLS PMD channel signals	$d[D_{PMD}, B_{PMD}]$	BU/s	t	-	
$\hat{S}$	Expected PMD channel signal as derived from the main channel signals for a given PMD dispersion.	$d[*, *, B_{PMD}]$ (dimensions depend on wavelength grid)	BU/s	t	-	
λ_{FPA}	Main channel wavelength grid	$d[D_{FPA}, B_{FPA}]$	nm	t	-	
λ_{MME}	Wavelength grid for Müller matrix elements	d[D,B]	nm	t	-	
$\delta\lambda_E$	Sampling interval for equidistant wavelength grid	d	nm	t	-	
λ_E	Equidistant wavelength grid	$d[N_E]$	nm	t	-	
c	Cross-correlation function	d[*]	-	t	-	
Δ	Spectral shift from current iteration for current PMD and current window	d	$\delta\lambda_E$	t	-	
h	Peak height of cross-correlation function for current PMD and current window	d		t	-	
δ	Total spectral shift from cross correlation algorithm, both PMDs, all windows	$d[N_w, B_{PMD}]$	nm	t	-	
B	The HWHM of the FFT of the cross-correlation function.	d	-	t	-	
r	Intermediate variable - see algorithm description.	d	-	t	-	
σ_a	Root mean square of the antisymmetric part of the cross-correlation function.	d	-	t	-	
ε	Error estimate for cross-correlation	$d[N_w, B_{PMD}]$		t	-	[RD 8]

5.2.16.3.3 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/Remarks*
$N_{\psi f}$	Number of viewing angles for which the fine viewing angle grid is specified	w	-	i	A2.01	
t_{stab}	Stabilisation time for SLS lamp	d	s	i	A2.01	
M	Order of wavelength calibration polynomial for channel	i [B]	-	i	A2.01	
N_w	Number of spectral windows for cross-correlation algorithm	i	-	i	A2.01	
λ_w	Start-/end wavelengths for spectral windows	$d[2, N_w]$	nm	i	A2.01	
$\lambda_{E, start}$	Start wavelength for equidistant wavelength grid	d	nm	i	A2.01	
$\lambda_{E, end}$	End wavelength for equidistant wavelength grid	d	nm	i	A2.01	
N_E	Number of points in equidistant wavelength grid	i	nm	i	A2.01	
Δ_{max}	Maximum spectral shift allowed for the calibration to be successful	$d[B_{PMD}]$	pixel	i	A2.01	
$N_{it,max}$	Maximum number of iterations allowed	$i[B_{PMD}]$	-	i	A2.01	
t_{gof}	Threshold for goodness of fit for PMD spectral calibration	$d[B_{PMD}]$	-	i	A2.01	
$\psi_{SM,0}$	Viewing angle at $n_{SM} = 0$	d	degree	i	A2.01	

5.2.16.3.4 Input from key dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
N_q	Number of Stokes fractions for SLS radiance at the output of the GOME-2 Calibration Unit	i	-	i	A2.0.4	
λ_{qc}	Wavelength grid associated with the Stokes fractions for SLS output of the GOME-2 Calibration Unit	d[N_q]	nm	i	A2.0.4	
q_c	Stokes fractions for SLS radiance at the output of the GOME-2 Calibration Unit	d[N_q]	-	i	A2.0.4	
N_{pix}	Maximum number of detector pixels for which PMD slit function is defined (for a given wavelength)	i	-	i	A2.0.4	
N_{wl}	Number of wavelengths for which the PMD slit function is given	i	-	i	A2.0.4	
λ_F	Wavelength for PMD slit function	d[N_{wl}]	nm	i	A2.0.4	
F	PMD slit function	d[N_{pix},N_{wl}]	-	i	A2.0.4	
λ_{OL}	Wavelength of main channel separation (50% / 50% intensity point)	d[3]	nm	i	A2.0.4	The elements will be referenced as $\lambda_{OL1\text{-}2}$, $\lambda_{OL2\text{-}3}$, $\lambda_{OL3\text{-}4}$ below
λ^{REF}_{PMD}	Reference PMD channel wavelength grid from key data.	d[D_{PMD}, B_{PMD}]	nm	i	A2.0.4	Used as a first-guess for iteration

5.2.16.3.5 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
a	Spectral calibration polynomial coefficients.	d[B, max(M)]	-	i	A2.13	Input: FPA coefficients (first index: 0…3)

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
pmd_transfer	PMD transfer mode	enum[N]		i	A2. 3	
M^1	Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D, B, $N_{\psi f}$]	BU.s^{-1}/(photons/ (s.cm^2.sr.nm))	i	A2.1	
μ^2	Ratio of MMEs M^2 to M^1 which describes the polarisation sensitivity of the instrument	d[D, B, $N_{\psi f}$]	-	i	A2.1	
ψ	Viewing angle for *SLS* observation mode.	d	degree	i	A2.3.1	
F_{SAA}	Flag indicating whether scan is in the SAA	bitstring [32,N]	-	i	A2.7	1 = in SAA 0 = not in SAA
S	SLS PMD channel signals (raw transfer mode), dark signal and PPG corrected and normalised on one-second integration time	d[D_{PMD},B_{PMD},N]	BU/s	i	A2.12	
$\bar{S}^{FPA}$	Averaged SLS main channel signals	d[D, B_{FPA}]	BU/s	i	A2.13	
missing	Mask indicating missing mean values	bool[D,B]	-	i	AX.1	1 = missing 0 = not missing

5.2.16.3.6 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
λ_{PMD}	Full spectral calibration grid for PMDs	d[B,D]	nm	o	ifc	
F_{noconv}	Flag indicating that PMD spectral calibration has not converged, per PMD channel	bool[B_{PMD}]	-	o	ifc	1 = not converged 0 = converged
N_{it}	Number of iterations	w[N_w, B_{PMD}]	-	o	ifc	
gof	Goodness of fit per PMD channel	d[B_{PMD}]	-	o	ifc	
F_{gof}	Flag indicating whether goodness of fit for PMD spectral calibration is above specified threshold	bool[B_{PMD}]	-	o	ifc	1 = goodness of fit too low 0 = goodness of fit acceptable

5.2.16.4 Algorithm

Prerequisite: Module Calculate Spectral Calibration Parameters for Main Channels (A2.13) must have been executed for the current SLS calibration sequence already.

If *pmd_transfer* = *raw* (i.e. PMD data is transferred in raw mode) the following calculations are carried out. Otherwise nothing is done for PMD channels.

5.2.16.4.1 Average Relevant SLS Measurements (A2.14.1)

Average PMD spectra S from one SLS calibration sequence using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1), excluding the measurements for a time period t_{stab}^{SLS} after lamp ignition as determined from the SLS current (see A2.13.1). This gives an averaged PMD spectrum $\bar{S}$. Average also the viewing angles for those measurements which went into the signal average. This yields an average viewing angle ψ_{SLS}. Scans for which F_{SAA} = 1 for any readout are excluded from the calculation of spectral calibration coefficients. In the case that there are detector pixels with no valid readouts in any channel as indicated by *missing*, no spectral calibration coefficients are generated for that channel.

5.2.16.4.2 Calculate Spectral Calibration Parameters (A2.14.2)

In contrast to the main channels, the PMD spectral calibration is performed on a full spectral grid. A polynomial representation is not used at any point.

The 256 detector pixels containing useful information in raw transfer mode are the ones from PMD blocks C, D, and E, corresponding to detector pixel numbers $i = 768 \ldots 1023$ (see Appendix B). All calculations below are performed on averaged SLS spectra.

5.2.16.4.2.1 Initialise

1. Obtain the main channel wavelength grid $\lambda_{FPA,ij}$ ($i = 0 \ldots Dj - 1$, $j = 1 \ldots B_{FPA}$) from a call to module Apply Spectral Calibration (AG.14) for the main channels, providing main channel polynomial coefficients a_{jm} ($j = 1 \ldots B_{FPA}$, $m = 0 \ldots M_j$) on input. These coefficients must have been derived in module Calculate Spectral Calibration Parameters for Main Channels (A2.13) using the same SLS calibration sequence.
2. Obtain the first guess PMD channel wavelength grid $\lambda_{PMD,ij}^{REF}$ ($i = 0 \ldots Dj - 1$, $j = 1 \ldots B_{PMD}$) from the key-data files WL_PMD_P_MON and WL_PMD_S_MON.
3. From the actual averaged viewing angle ψ_{SLS} (looking *inside* the instrument), calculate an equivalent viewing angle ψ within the viewing angle range covered by the calibration key data, i.e., looking *outside* the instrument.

   Note: ψ_{SLS} and ψ are equivalent in the sense that the incidence angles on the scan mirror are the same for both viewing angles.

$$\psi = 2\left|\psi_{SM,0}\right| - \psi_{SLS} \qquad \textit{Equation 95}$$

4. Interpolate main channel and PMD Müller matrix elements $M^1(\lambda_{MME,ij})$ and $\mu^2(\lambda_{MME,ij})$ from the fine viewing angle grid to the equivalent SLS angle ψ, using Linear Interpolation (AX.2) to yield $M^1_\Psi(\lambda_{MME,ij})$ and $\mu^2_\Psi(\lambda_{MME,ij})$ ($i = 0\ldots Dj - 1$, $j = 1\ldots B$).
5. Interpolate main channel Müller matrix elements $M^1_\Psi(\lambda_{MME,ij})$ and $\mu^2_\Psi(\lambda_{MME,ij})$ ($i = 0\ldots Dj - 1$, $j = 1\ldots B_{FPA}$) from their wavelength grid to that of the SLS main channel data $\lambda_{FPA,ij}$ using Spline Interpolation (AX.3) to yield $M^1_{\Psi,FPA}(\lambda_{FPA,ij})$ and $\mu^2_{\Psi,FPA}(\lambda_{FPA,ij})$ ($i= 0\ldots D_j - 1$, $j = 1\ldots B_{FPA}$). For spectral points of $\lambda_{FPA,ij}$ outside the wavelength grid of the Müller matrix elements set $M^1_{\Psi,FPA}(\lambda_{FPA,ij})$ and $\mu^2_{\Psi,FPA}(\lambda_{FPA,ij})$ equal to the first (or last) valid value on the original wavelength grid.
6. Interpolate SLS Stokes fractions q_c from their wavelength grid to that of the SLS main channel data $\lambda_{FPA,ij}$ using Spline Interpolation (AX.3) to yield $q_c(\lambda_{FPA,ij})$. For spectral points of $\lambda_{FPA,ij}$ outside the wavelength grid of q_c, set $q_c(\lambda_{FPA,ij})$ equal to the first (or last) valid value on the original wavelength grid.
7. Correct the main channel SLS spectrum for radiance and polarisation sensitivity:

$$\hat{S}^{FPA}_{ij} = \frac{\overline{S^{FPA}_{ij}}}{M^1_{\psi,FPA}(\lambda_{FPA,ij})(1 + \mu^2_{\psi,FPA}(\lambda_{FPA,ij}) \cdot q_c(\lambda_{FPA,ij}))}$$ *Equation 96*

8. Concatenate $\lambda_{FPA,ij}$ and $\hat{S}^{FPA}_{ij}$ for the main channels as follows:
   FPA 1 ($j = 1$): Use elements i such that $\lambda_{FPA,ij} < \lambda_{OL1-2}$
   FPA 2 ($j = 2$): Use elements i such that $\lambda_{OL1-2} < \lambda_{FPA,ij} < \lambda_{OL2-3}$
   FPA 3 ($j = 3$): Use elements i such that $\lambda_{OL2-3} < \lambda_{FPA,ij} < \lambda_{OL3-4}$
   FPA 4 ($j = 4$): Use elements i such that $\lambda_{OL3-4} < \lambda_{FPA,ij}$

   This reduces the number of dimensions of $\lambda_{FPA,ij}$ and $\hat{S}^{FPA}_{ij}$ by one to $\lambda_{FPA,i}$ and $\hat{S}^{FPA}_{i}$.
9. Create the equidistant wavelength grid. The number of points in the equidistant wavelength grid is given by the following:

$$\delta\lambda_E = \frac{\lambda_{E,end} - \lambda_{E,start}}{N_E - 1}$$ *Equation 97*

and the grid points are defined by

$$\lambda_{E,k} = \lambda_{E,start} + k \cdot \delta\lambda_E \qquad (k = 0\ldots N_E - 1)$$ *Equation 98*

10. Interpolate FPA signals $\hat{S}_i^{\mathrm{FPA}}$ and PMD signal $\hat{S}$ to the equidistant grid $\lambda_{E,k}$ using Spline Interpolation (AX.3). For spectral points of $\lambda_{E,k}$ outside the wavelength grid of $\hat{S}_i^{\mathrm{FPA}}$ or $\hat{S}$ set the interpolated values equal to the first (or last) valid point on the original wavelength grid.
11. Initialise spectral shifts δ_{nw} (n = s, p; $w = 0\ldots N_w-1$) to zero.
12. Convolve $\hat{S}^{\mathrm{FPA}}(\lambda_{E,k})$ with the PMD slit function F, yielding $\hat{S}_n^{\mathrm{FPA,conv}}(\lambda_{E,k})$ (n = 5...6) taking into account the variation of the PMD slit function with wavelength. Follow steps a-g listed below:
    a. For each of the N_{wl} spectral points for which the PMD slit function is given, determine the start/end wavelengths for the slit function, i.e., the wavelengths corresponding to the first and last detector pixel for which the PMD slit function is given using the first guess PMD channel wavelength grid $\lambda_{\mathrm{PMD},ij}$ from step 2.
    b. For each of the N_{wl} spectral points for which the PMD slit function is given, determine the index in the equidistant wavelength grid corresponding to the start/end wavelengths from step a. and the centre-of-gravity wavelength λ_F using a subroutine such as `hunt`of [RD 9].
    c. For each of the N_{wl} spectral points for which the PMD slit function is given, interpolate the PMD slit function from its grid to the equidistant wavelength grid using the start/end indices from step b and using Spline Interpolation (AX.3).
    d. Of the N_{wl} resulting interpolated PMD slit functions from step c., find the one which covers the maximum number of equidistant grid pixels. Use this number for array sizing in the following steps.
    e. Re-index interpolated PMD slit functions from step c. such that they are all aligned at their centre-of-gravity. Use index 0 for the centre-of-gravity.
    f. For all grid points in the equidistant grid calculate a slit function corresponding to the respective grid point by interpolation of the aligned interpolated PMD slit functions from step e. using Linear Interpolation (AX.2).
    g. Convolve $\hat{S}^{\mathrm{FPA}}(\lambda_{E,k})$ with the PMD slit function by applying for each grid point the slit function from step f., resulting in a convolved main channel SLS spectrum $\hat{S}_n^{\mathrm{conv}}(\lambda_{E,k})$.
13. Interpolate $M^1_{\Psi,\mathrm{PMD},n}$, $\mu^2_{\Psi,\mathrm{PMD},n}$, and q_c to the equidistant grid $\lambda_{E,k}$ using Spline Interpolation (AX.3). For spectral points of $\lambda_{E,k}$ outside the wavelength grid of $M^1_{\Psi,\mathrm{PMD},n}$, $\mu^2_{\Psi,\mathrm{PMD},n}$, or q_c set the interpolated values equal to the first (or last) valid point on the original wavelength grid.
14. Convert the convolved main channel SLS spectrum to the spectrum the PMD channel would observe, correcting for different radiance and polarisation sensitivities in the PMD channel:

$$\hat{S}_n^{\mathrm{conv}}(\lambda_{E,k}) = [M^1_{\Psi,\mathrm{PMD},n}(\lambda_{E,k})(1+\mu^2_{\Psi,\mathrm{PMD},n}(\lambda_{E,k})\cdot q_c(\lambda_{E,k}))]\hat{S}_n^{\mathrm{FPA,conv}}(\lambda_{E,k}) \qquad \text{Equation 99}$$

where $k = 0\ldots N_E - 1$, n = 5...6.

5.2.16.4.2.2 Iterate

Loop information: The following steps are performed for both PMD channels n = s, p and for all PMD spectral windows $w = 0\ldots N_w - 1$.

15. Determine cross-correlation c between convolved FPA spectrum $\hat{S}_n^{\mathrm{conv}}(\lambda_{E,k})$ and PMD spectrum $\bar{S}_n(\lambda_{E,k})$. A cross-correlation algorithm such as the subroutine `correl` of [RD 9] shall be used. Determine the position Δ and height h of the maximum of the cross-correlation function. Δ is the spectral shift of the PMD spectrum with respect to the FPA spectrum in units of the equidistant grid spacing $\delta\lambda_E$. We use the following sign convention: Δ is positive if the PMD spectrum is shifted to greater wavelengths compared to the FPA spectrum, i.e., if

$$\hat{S}_n^{\mathrm{conv}}(\lambda_{E,k}) = \bar{S}_n(\lambda_{\mathrm{E},k+\Delta})$$

Equation 100

16. Update the total spectral shift δ_{nw} by adding $\Delta \times \delta\lambda_E$. Update the PMD wavelength grid accordingly.
17. If the spectral shift Δ is still above given threshold $\Delta_{\max,n}$ and the number of iterations $N_{it,nw}$ is less than $N_{it,max}$, start next iteration (at 15.). Otherwise we are done.

End of loop

5.2.16.4.2.3 Finalise

18. Recalculate cross-correlation function c with the final spectral shift applied and recalculate the position Δ and height h of the maximum of the cross-correlation function.
19. Calculate the cross-correlation error ε_{nw} as $\varepsilon_{nw} = \frac{1}{4} \times \frac{N}{2B} \times \frac{\delta\lambda_E}{1+r}$ where N is the number of pixels in the spectral window, B is the half-width half-maximum of the peak of the real part of the discrete Fourier transform of the cross-correlation function (from the last iteration), and $r = \frac{h}{\sqrt{2}\sigma_a}$, with σ_a denoting the root-mean-square of the anti-symmetric part of the cross correlation function c (with peak at c_0) [RD 8], $\sigma_a = \sqrt{\frac{1}{N}\sum_n (c_n - c_{-n})^2}$. In order to calculate the discrete Fourier transform the cross-correlation function has to be in wrap-around order–the negative branch is completely shifted to the far side of the positive branch.
20. For each PMD channel n, perform linear fit to the retrieved spectral shifts δ_{nw} ($w = 0\ldots N_w - 1$), using a least squares fit (χ^2 minimisation using singular value decomposition) with cross-correlation errors ε_{nw} as standard deviations (values) input (i.e., use $1/(\varepsilon_{nw})^2$ as error weights), yielding two coefficients per PMD channel. The χ^2 from this fit is taken as goodness-of-fit (gof_n) for the PMD spectral calibration.

21. For each PMD channel n, calculate the pixel shift Δ_{in} per detector pixel from the two coefficients obtained in the previous step. Calculate a new wavelength axis using this pixel shift:

$$\tilde{\lambda}_{PMD,\,in} = \lambda_{PMD,\,in} + \Delta_{in}\delta\lambda_E \quad \text{Equation 101}$$

5.2.16.4.3 Determine PCDs From PMD Spectral Calibration (A2.14.3)

Assuming F_{conv} and F_{gof} have been initialised to zero, then for $n = 1...B_{PMD}$ if

$$N_{iter,\,n} = N_{it,\,max} \quad \text{Equation 102}$$

and one of the iterations has not converged, set

$$F_{noconv,\,n} = 1 \quad \text{Equation 103}$$

If the 'Goodness of Fit' of the PMD spectral calibration is larger than $t_{gof,n}$ then set

$$F_{gof,\,n} = 1 \quad \text{Equation 104}$$

5.2.17 APPLY SPECTRAL CALIBRATION PARAMETERS (A2.15)

Instrument Modes		Instrument Data	
Earth (PMD only)	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS	√		
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Apply Spectral Calibration (AG.14)

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.2.18 CALCULATE ETALON CORRECTION (A2.16)

Instrument Modes		**Instrument Data**	
Earth		PMD	√
Dark		FPA	√
Sun		Housekeeping	
WLS	√		
SLS			
SLS over Diffuser			
LED			
Moon			

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1)
Linear Interpolation (AX.2)
Spline Interpolation (AX.3)

Data Granule

All scans from on LED calibration mode measurement period.

5.2.18.1 Objectives

To calculate an Etalon correction using measurements taken in the *WLS* calibration mode.

5.2.18.2 Description

Etalon is an interference phenomenon, which arises in the thin protective layer coated on the detector chip. This causes a wave-like pattern on the radiance response, where the position of the minima and maxima of the wave depend on the ratio between layer thickness and wavelength. At the shortest wavelengths in channel 1 we expect (based on ERS-2/GOME experience) approximately 10 minima and maxima over the channel (i.e. the interference wave has a wavelength of approximately 100 pixels). At the longest wavelengths of the channel 4 this number reduces proportionally with wavelength to around 4 (250 pixels per interference wavelength).

A variable etalon arises when condensates (ice) settle on the detector, thereby effectively increasing the thickness of the interference layer. This causes a shift of the interference pattern with respect to that calibrated on ground. Since the radiance response function measured in the on-ground calibration already contains the static part of the etalon, it is only necessary to correct for the differential variable etalon caused by condensates in orbit.

The measured WLS detector signal readouts are corrected for dark signal, normalised to one-second integration time, corrected for PPG and spectrally calibrated. PMD data are assumed to be transferred in raw transfer mode. If this is not the case PMD data are excluded from the calculations. To maximise the signal-to-noise ratio in the WLS measurements a mean spectrum is calculated from all measurements obtained during one *WLS* calibration mode period, excluding the measurements for a time period t_{stab}^{wls} after lamp switch-on as determined from the WLS current.

The mean WLS spectrum is divided by a reference WLS spectrum measured as part of the on-ground calibration. The latter has the same etalon as the radiance response function from the on-ground calibration. This reference WLS spectrum, after correction for PPG using the on-ground PPG characterisation, must be interpolated to the wavelength of the measured WLS spectrum. It is assumed that changes in spectral calibration over one orbit are small enough with respect to the etalon frequency that they can be neglected. Therefore only one spectral calibration is required.

The first algorithm described below uses a Fourier-filter to select only those frequencies which can be assigned to etalon. It is necessary to begin with spectra which are as far as possible normalised to a flat spectrum oscillating around the baseline (an ‘AC signal’). It is also required that only reliable signals are used to avoid the introduction of rogue features in the Fourier frequency domain. To this end, the initialisation data prescribes for each channel the start and end pixel of the spectral region to be used in each channel. Theoretical modelling of etalon shows that Etalon frequency is linear with inverse wavelength, implying that a clean Fourier spectrum can only be obtained if the spectrum is first re-binned to an inverse wavelength scale. The second algorithm assumes that the instrument in-orbit radiometric response at time t, as described in Appendix E, can be corrected for deviations from the on-ground characterisation using the ratio of the mean WLS detector readouts to the reference WLS measurements obtained during on-ground calibration. In the case of failure of the WLS lamp, the etalon correction may be calculated using the Solar Mean Reference spectrum in place of the mean WLS measurements.

The channel mean and standard deviation of the residuals not accounted for by the etalon correction are calculated as diagnostic quantities. The remaining structures on a pixel level, *cppg*, are determined by smoothing the residual spectrum over a number of pixels, using a triangular smoothing function. The channel mean and standard deviation of *cppg* are also stored as diagnostic quantities. If any of these diagnostic quantities exceed threshold values specified in the initialisation dataset a flag is raised.

Note: WLS measurements taken in regions with a high background of cosmic rays such as the South Atlantic Anomaly (SAA) described in Section 5.7.8, shall be excluded from calibration processing.

5.2.18.3 Variables

5.2.18.3.1 *Local Variables*

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	References/Remarks
k	Detector pixel index counter	i	-	t	-	
N	Total number of scans to be accumulated and averaged.	i	-	t	-	
WLS_{ratio}	Ratio of mean to reference WLS spectra	d[D,B]	-	t	-	
LIN	Quadratic baseline to be removed from WLS_{ratio} taking into account the 1 g to 0 g effect in the lamp.	d[NET, B]	-	t	-	
SB	Basis spectrum	d[D,B]	-	t	-	
SB^{rebin}	Basis spectrum rebinned to uniform inverse wavelength grid	d[NET, B]	-	t	-	
SB^{FFT}	Fourier transform of basis spectrum	d[NET, B]	-	t	-	
P	Filter function	d[NET, B]	-	t	-	
FIL	Result of filtering the Fourier transform of the basis spectrum	d[NET, B]	-	t	-	
ETN^{rebin}	Etalon correction on the uniform inverse wavelength grid	d[NET, B]	-	t	-	
RES	Residual etalon	d[D,B]	-	t	-	
RES^{sm}	Smoothed residual spectrum	d[D,B]	-	t	-	
$cppg$	Spectrum of residual structure at a pixel level	d[D,B]	-	t	-	
v	Inverse wavelength grid	d[D,B]	$0.0003 \times cm^{-1}$	t	-	
v^{regrid}	Inverse wavelength grid regridded to uniform spacing	d[D,B]	$0.0003 \times cm^{-1}$	t	-	
δ	Interval on inverse wavelength grid for regridding	d[B]	$0.0003 \times cm^{-1}$	t	-	
δ_p	Interval on inverse wavelength grid for regridding	d	$0.0003 \times cm^{-1}$	t	-	
δ_m	Interval on inverse wavelength grid for regridding	d	$0.0003 \times cm^{-1}$	t	-	

5.2.18.3.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
Eta_algo	Etalon correction algorithm selection	enum	-	i/o	A2.0.1/ifc	
Eta_back	Switch for selection of backup source (SMR) in event of WLS failure	enum	-	i/o	A2.0.1/ifc	
ETS	Start detector pixel for each channel for use in Etalon correction calculation	i[B]	-	i	A2.0.1	
ETE	End detector pixel for each channel for use in Etalon correction calculation	i[B]	-	i	A2.0.1	
t_{stab}^{WLS}	Stabilisation time for WLS lamp	d	s	i	A2.0.1	
f	Fourier frequencies used to determine filter *P* for each channel.	i[4,B]	-	i	A2.0.1	Four frequencies are specified per channel.
s_{PPG}	Smoothing width	i	pixel	i	A2.0.1	Must be odd
$t_{\overline{RES}}$	Threshold for mean residual etalon per channel	d[B]	-	i	A2.0.1	
$t_{\sigma RES}$	Threshold for standard deviation of residual etalon per channel	d[B]	-	i	A2.0.1	
$t_{\overline{PPG}}$	Threshold for residual pixel level structure per channel	d[B]	-	i	A2.0.1	
$t_{\sigma PPG}$	Threshold for standard deviation of residual pixel level structure per channel	d[B]	-	i	A2.0.1	

5.2.18.3.3 Input from key dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
WLS_{ref}	Reference WLS detector readouts, corrected for PPG	d[D,B]	BU/s	*i*	A2.0.4	
λ_{ref}	Wavelength grid associated with the reference WLS measurements	d[D,B]	nm	*i*	A2.0.4	
SMR_{ref}	Reference SMR spectra, corrected for PPG	d[D,B]	photons/(s.cm^2.nm)	*i*	A2.0.4	
λ_{SMref}	Wavelength grid associated with the reference SMR measurements	d[D,B]	nm	*i*	A2.0.4	
$i_{\mathrm{valid,start}}$	Start pixel of valid data per channel	d[D]	-	*i*	A2.0.4	
$i_{\mathrm{valid,end}}$	End pixel of valid data per channel	d[D]	-	*i*	A2.0.4	

5.2.18.3.4 Input/output from other functions

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/ Remarks*
UTC_{WLS}	UTC date/time of *WLS* (or *Sun* if *Eta_back* = *Sun*) calibration mode measurements	d[N]	fractional days	*i*	A2.3	
pmd_transfer	PMD transfer mode	enum[N]	-	*i*	A2.3	
F_{SAA}	Flag indicating whether scan is in the SAA	bit-string [32,N]	BU/s	*i*	A2.7	1 = in SAA 0 = not in SAA
WLS	Detector readout values from *WLS* calibration mode, corrected for dark signal and PPG, normalised to an integration time of one second.	d[D,B, N]	BU/s	*i*	A2.12	
$\overline{WLS}$	Mean WLS detector readouts.	d[D,B]	-	*i*	AX.1	
missing	Mask indicating missing mean values	i[D,B]	-	*i*	AX.1	1 = missing 0 = not missing

5.2.18.3.5 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
WLS_{start}	Start UTC date/time of valid *WLS* (or *Sun* if *Eta_back* = *Sun*) calibration mode measurements	d	fractional days	o	ifc	
WLS_{end}	End UTC date/time of valid *WLS* (or *Sun* if *Eta_Back* = *Sun*) calibration mode measurements	d	fractional days	o	ifc	
λ^{ETN}	Wavelength grid for the measurements from *WLS* calibration mode and the Etalon correction	d[D,B]	nm	i/o	A2.15/ifc	
ETN	Etalon correction	d[D,B]	BU/s	o	ifc	
$\overline{RES}$	Mean residual etalon per channel	d[B]	-	o	ifc	
σ_{PPG}	Standard deviation of residual etalon per channel	d[B]	-	o	ifc	
$\overline{cppg}$	Mean residual structure at a pixel level	d[B]	-	o	ifc	
σ_{cppg}	Standard deviation of residual structure at a pixel level	d[B]	-	o	ifc	
$F_{\overline{RES}}$	Flag indicating whether mean residual etalon exceeds specified threshold per channel	bool[B]	-	o	ifc	1 = exceeds 0 = does not
$F_{\sigma RES}$	Flag indicating whether standard deviation of residual etalon exceeds specified threshold per channel	bool[B]	-	o	ifc	1 = exceeds 0 = does not
$F_{\overline{cppg}}$	Flag indicating whether mean residual pixel level structure exceeds specified threshold per channel	bool[B]	-	o	ifc	1 = exceeds 0 = does not
$F_{\sigma_{cppg}}$	Flag indicating whether standard deviation in residual pixel level structure exceeds specified threshold per channel	bool[B]	-	o	ifc	1 = exceeds 0 = does not
F_{Eta}^{miss}	Flag indicating that missing mean *WLS* calibration mode measurements have been filled by interpolation or that one complete channel is missing	enum[B]	-	o	ifc	

5.2.18.4 Algorithm

If *pmd_transfer* = *raw* (i.e. PMD data is transferred in raw mode) the following calculations are carried out for both main and PMD channels. Otherwise the calculations are carried out for main channels only. Nothing is done for PMD channels. Note also that etalon correction is calculated per channel. Main channel bands need only be separated for the calculation of a mean WLS readout. Furthermore, the spectral calibration can be assumed to be constant during one WLS calibration mode period. Before proceeding first calculate:

$$NET = ETE - ETS + 1 \quad \text{Equation 105}$$

If for a given channel $ETS < i_{\mathrm{valid,start}}$ then set $ETS = i_{\mathrm{valid,start}}$ and raise a warning via the MCS. Similarly, if $ETE > i_{\mathrm{valid,end}}$ then set $ETE = i_{\mathrm{valid,end}}$ and raise a warning via the MCS.

5.2.18.4.1 Calculate Mean of all WLS Readouts (A2.16.1)

The mean WLS, dark signal and PPG corrected detector readout, and the noise in the mean are calculated according to Section 5.8.1, excluding the measurements for a time period t_{stab}^{WLS} after lamp switch-on as determined from the WLS current (switch-on defined as the time when the WLS current exceeds I_{low}^{WLS} for the first time). The data has previously been checked for saturated pixels and hot pixels using Determine PCDs from Raw Intensity (A2.4). Note that WLS measure *cppg* measurements taken in regions with a high background of cosmic rays such as the South Atlantic Anomaly (SAA) as described in Section 5.7.8, shall be excluded from calibration processing.

Any detector pixels for which there are no valid readouts, as indicated by *missing*, are assigned mean values which are equal to a linear interpolation between the nearest valid neighbouring values calculated using Linear Interpolation (AX.2). In the case that an entire channel is missing, no etalon correction is calculated for that channel.

5.2.18.4.2 Prepare WLS Basis Spectrum for Etalon Correction (A2.16.2)

- Interpolate WLS_{ref} onto the wavelength grid of $\overline{WLS}$ using Spline Interpolation (AX.3) yielding $WLS_{ref}(\lambda^{ETN})$
- For $i = 0...D_j - 1$, $j = 1...B$ calculate the ratio:

$$WLS_{ratio}(\lambda^{ETN}{}_{ij}) = \overline{WLS}(\lambda^{ETN}{}_{ij}) / WLS_{ref}(\lambda_{ij}^{ETN}) \quad \text{Equation 106}$$

- For $j = 1...B$, calculate LIN_{ij} by least-square-fitting a quadratic function to WLS_{ratio} between ETS_j and ETE_j, i.e., minimise:

$$\sum_{i = ETS_j}^{ETE_j} (LIN_{ij} - WLS_{ratio,\,ij})^2 \text{ where } LIN_{ij} = a_j i + b_j . \quad \text{Equation 107}$$

Singular value decomposition shall be used for the fit.

- For $i = ETS_j ... ETE_j$ and $j = 1...B$, calculate the basis spectrum as follows:

$$SB_{ij} = WLS_{ratio,\, ij} / LIN_{ij} \text{ and}$$ *Equation 108*

$$SB_{ij} = 1 \text{ for } i = 1...ETS_j - 1 \text{ and } i = ETN_j + 1...D_j$$ *Equation 109*

5.2.18.4.3 Calculate Etalon Correction (A2.16.3)

5.2.18.4.3.1 ALGORITHM OPTION 1: (A2.16.3.1)

If *Eta_algo = Algo1* then calculate the etalon correction using the following algorithm:

- Assign an inverse wavelength scale for $i = ETS_j...ETE_j$, and $j = 1...B$ defined by:

$$\nu_{ij} = 3000 / (\lambda^{ETN}{}_{ij})$$ *Equation 110*

- Regrid the inverse wavelength grid to be equally spaced such that for $i = ETS_j...ETE_j$ and $j = 1...B$. The inverse wavelength grid is descending, however the regridding is carried out in such a way that the equally spaced grid will be ascending.

$$\nu_{ij}^{regrid} = \nu_{ETE_j\, j} + (i - ETS_j) \cdot \delta_j \text{ where}$$ *Equation 111*

$$\delta_j = \frac{\nu_{ETS_j\, j} - \nu_{ETE_j j}}{ETE_j - ETS_j}$$ *Equation 112*

- Rebin the basis spectra to the regridded inverse wavelength grid such that for $i = ETS_j...ETE_j$ and $j = 1...B$ calculate:

$$SB_{ij}^{rebin} = \frac{1}{\sum k} \cdot \sum SB_{kj}$$ *Equation 113*

for those values of k which satisfy the following:

$$\nu_{ij}^{regrid} - \delta_j / 2 < \nu_{kj} \le \nu_{ij}^{regrid} + \delta_j / 2$$ *Equation 114*

For i such that no values ν_{kj} of satisfy Equation 114, SB_{ij}^{rebin} is calculated by linear interpolation between $SB_{(i\,-1)j}^{rebin}$ and $SB_{(i\,+-1)j}^{rebin}$ as described in Linear Interpolation (AX.2).

- Calculate a Discrete Fourier Transform of the rebinned basis spectrum as follows:

$$SB_{nj}^{FFT} = \sum_{i=0}^{NET_j - 1} (SB_{(i+ETS_j)j}^{rebin} - 1) \cdot e^{2\pi Ini/(NET_j)}$$ *Equation 115*

where $I = \sqrt{-1}$ and $n = 0 \ldots NET_j - 1$ are the Fourier frequencies. *Equation 116*

It is recommended that for implementation of the discrete Fourier Transform calculation, a Fast Fourier transform algorithm such as the Cooley-Tukey algorithm should be considered.

- The discrete Fourier transform of the rebinned basis spectrum is filtered for $n = 0...NET_j/2$ and as $j = 1...B$ as:

$$FIL_{nj} = P_{nj}(SB_{nj}^{FFT}) \text{ where}$$ *Equation 117*

$$P_{nj} = \begin{cases} 0 & for & n < f_{0j} \\ a_1 \cdot n + b_1 & for & f_{0j} \le n < f_{1j} \\ 1 & for & f_{1j} \le n \le f_{2j} \\ \cos(a_2 \cdot n + b_2) & for & f_{2j} < n \le f_{3j} \\ 0 & for & f_{3j} < n \end{cases} \text{ and}$$ *Equation 118*

$$a_1 = \frac{1}{(f_{1j} - f_{0j})} \text{ and } b_1 = -\frac{f_{0j}}{(f_{1j} - f_{0j})}$$ *Equation 119*

$$a_2 = \frac{\pi}{2 \cdot (f_{3j} - f_{2j})} \text{ and } b_2 = -f_{2j} \cdot \frac{\pi}{2 \cdot (f_{3j} - f_{2j})}$$ *Equation 120*

The Fourier frequencies f_{0j}, f_{1j}, f_{2j}, f_{3j} will be provided in the initialisation dataset and based on results from the on-ground calibration.

Note: If a complex-to-complex FFT formulation is used (with imaginary part zero) an array of size *NET* including both positive and negative frequencies is produced. The filter should then be applied to both the positive and negative frequency halves symmetrically, taking advantage of the complex conjugate symmetry, before creating an inverse transform. In the case that a real-to-complex formulation is used (and therefore the complex conjugate symmetry is implied) the FFT produces an array of size (*NET*/2) + 1 containing only the positive frequencies and the filter should be applied to this array directly.

- Apply an inverse discrete Fourier transform to be the filtered spectrum for $i = ETS_j ... ETE_j$ and $j = 1...B$ as follows:

$$FFT^{-1}(FIL_{ij}) = \frac{1}{NET_j} \cdot \sum_{n=0}^{NET_j - 1} FIL_{ij} \cdot e^{2\pi Ini/NET_j}$$ *Equation 121*

yielding the Etalon correction as:

$$ETN^{rebin}{}_{ij} = 1 + FFT^{-1}(FIL_{ij})$$ *Equation 122*

- The Etalon correction spectrum must be rebinned back to the original wavelength grid such that for $i = ETS_j ... ETE_j$ and $j = 1...B$ calculate:

$$ETN_{ij} = \frac{1}{\sum k} \cdot \sum ETN^{rebin}{}_{kj}$$ *Equation 123*

for those values of *k* which satisfy:

$$\nu_{ij} - \delta_{mi} < \nu_{kj}^{regrid} \le \nu_{ij} + \delta_{pi} \text{ where}$$
$$\delta_{pi} = (\nu_{ij} - \nu_{(i+1)j})/2$$
$$\delta_{mi} = (\nu_{(i-1)j} - \nu_{ij})/2 \text{ and}$$
$$\text{for } i = ETS_j + 1 ... ETE_j - 1 \text{ with}$$
$$\delta_{pETS_j} = \delta_{mETS_j} = ((\nu_{ETS_j j} - \nu_{(ETS_j+1)j})/2) \text{ and}$$
$$\delta_{pETE_j} = \delta_{mETE_j} = (\nu_{(ETE_j-1)j} - \nu_{ETE_j j})/2$$ *Equation 124*

For *i* such that no values of ν_{kj}^{regrid} satisfy Equation (124), ETN_{ij} is calculated by linear interpolation between $ETN_{(i-1)j}$ and $ETN_{(i+1)j}$ as described in Linear Interpolation (AX.2).

- For $i = 0 \ldots ETS_j - 1$, $i = ETE_j + 1 \ldots D_j - 1$, and $j = 1 \ldots B$:

$$ETN_{ij} = 1 \qquad \text{Equation 125}$$

5.2.18.4.3.2 ALGORITHM OPTION 2: (A2.16.3.2)

If *Eta_algo* = *Algo2* then calculate the etalon correction using the following algorithm.
For $i = 0 \ldots D_j - 1$ and $j = 1 \ldots B$:

$$ETN_{ij} = SB(\lambda^{ETN}{}_{ij}) \qquad \text{Equation 126}$$

For algorithm option 2, the etalon outside the valid range of the key data as indicated by $i_{valid,start}$ and $i_{valid,end}$ is set equal to one. Additionally, all PCDs are set to undefined and PCD flags are set to zero.

5.2.18.4.3.3 BACKUP ALGORITHM: CALCULATE ETALON CORRECTION FROM SOLAR SPECTRUM (A2.16.4)

If *Eta_back* = *Sun* then calculate the etalon correction using the SMR spectrum from the in-flight calibration data. The specific algorithm to be used is indicated by *Eta_algo* as described above with the exception that $\overline{WLS}$ is replaced by *SMR* and WLS_{ref} is replaced by SMR_{ref} . A reference solar spectrum is derived off-line after launch and is included in the key data set.

5.2.18.4.4 Determine PCDs from Etalon Correction (A2.16.5)

- The residual spectrum is calculated from the basis spectrum for $i = ETS_j \ldots ETE_j$, $j = 1 \ldots B$ as follows:

$$RES_{ij} = ETN_{ij} - SB_{ij} \qquad \text{Equation 127}$$

Outside, for $i = 0 \ldots ETS_j - 1$ and $i = ETE_j + 1 \ldots D_j$, $j = 1 \ldots B$, set:

$$RES_{ij} = 0 \qquad \text{Equation 128}$$

Then for $j = 1 \ldots B$:

$$\overline{RES}_j = \sum_{i = ETS_j}^{ETE_j} \frac{RES_{ij}}{NET_j} \text{ and } \sigma_{RES,j} = \sqrt{\frac{1}{ETE_j - ETS_j} \cdot \sum_{i = ETS_j}^{ETE_j} (RES_{ij} - \overline{RES}_j)^2} \qquad \text{Equation 129}$$

Assuming $F_{\overline{RES}}$ and $F_{\sigma RES,j} - 1$ have been initialised to zero, then if

$$|\overline{RES}_j| > t_{\overline{RES},j} \text{ then } F_{\overline{RES},j} = 1 \qquad \text{Equation 130}$$

and if

$$\sigma_{RES,j} > t_{\sigma_{RES},j} \text{ then } F_{\sigma_{RES},j} = 1$$ *Equation 131*

- Furthermore residual structures on a pixel level *cppg* are subsequently calculated as follows. The residual spectrum *RES* is smoothed using a triangular smoothing function of width s_{PPG} such that for $i = s_{PPG}...D_j - 1 - s_{PPG}$ and $j = 1...B$:

$$RES^{sm}_{ij} = \frac{1}{(s_{PPG})^2} \cdot \left(\sum_{k=-s_{PPG}}^{s_{PPG}} (s_{PPG} - |k|) \cdot RES_{(i+k),j} \right)$$ *Equation 132*

The residual structures on a pixel level are calculated for $i = s_{PPG}...D_j - 1 - s_{PPG}$ and $j = 1...B$:

$$cppg_{ij} = RES_{ij} - RES^{sm}{}_{ij}$$ *Equation 133*

For $i = 0...s_{PPG} -1$, $i = D_J - s_{PPG}...D_j -1$ and $j = 1...B$:

$$RES^{sm}_{ij} = RES_{ij}$$ *Equation 134*

$$cppg_{ij} = 0$$ *Equation 135*

Then for $j = 1...B$

$$\overline{cppg_j} = \sum_{i=ETS_j}^{ETE_j} \frac{cppg_{ij}}{NET_j} \text{ and } \sigma_{cppg,j} = \sqrt{\frac{1}{ETE_j - ETS_j} \cdot \sum_{i=ETS_j}^{ETE_j} (cppg_{ij} - \overline{cppg_j})^2}$$ *Equation 136*

Assuming $F_{\overline{cppg}}$ and $F_{\sigma_{cppg}}$ have been initialized to zero then if

$$|\overline{cppg_j}| > t_{\overline{cppg},j} \text{ then } F_{\overline{cppg},j} = 1$$ *Equation 137*

and if

$$\sigma_{cppg,j} > t_{\sigma_{cppg},j} \text{ then } F_{\sigma_{cppg},j} = 1$$ *Equation 138*

Finally, set $F^{miss}_{Eta,j}$ to:

- *some_missing* if interpolated values were included in the mean signals for channel *j* as a result of missing mean values,
- *all_missing* if the entire channel *j* is missing,
- *no_missing* otherwise.

5.2.19 APPLY ETALON CORRECTION (A2.17)

Instrument Modes		Instrument Data	
Earth		PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Apply Etalon Correction (AG.14)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan.

5.2.20 DETERMINE STRAY LIGHT CORRECTION (A2.18)

Instrument Modes		Instrument Data	
Earth (PMD only)	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Determine Stray light Correction (AG.15)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan.

5.2.21 APPLY STRAY LIGHT CORRECTION (A2.19)

Instrument Modes		Instrument Data	
Earth (PMD only)	√	PMD	√

Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Apply Stray light Correction (AG.17)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan.

5.2.22 CALCULATE SMR (A2.20)

Instrument Modes		Instrument Data	
Earth		PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			

Uses Generic Sub-Function:

Apply Spectral Calibration (AG.14)

Apply Irradiance Response (AG.18)

Correct Doppler Shift (AG.19)

Uses Auxiliary Sub-Functions:

Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1)

Linear Interpolation (AX.2)

Spline Interpolation (AX.3)

Data Granule

All scans from one *Sun* observation mode measurement period.

5.2.22.1 Objectives

To calculate a Solar Mean Reference spectrum (SMR) on the basis of detector readouts measured during *Sun* observation mode.

5.2.22.2 Description

GOME-2 measures solar spectra during *Sun* observation mode (see Section 2.3.3). An on-board diffuser is placed in the light path during *Sun* observation mode to scatter the collimated solar irradiance into a diffuse radiance beam. During the *Sun* observation mode, the Sun moves through the FOV of the diffuser in elevation direction. The solar azimuth angle does not change significantly during the time interval of Sun observation, but depends on season. The solar calibration timeline will start before the Sun is fully in the field-of-view of the diffuser, and end after the Sun has left the FOV. Only those detector readouts for which the Sun is fully in the FOV are used in the calculation of the SMR. Selection is based on solar elevation angle. Only those measurements within a pre-specified range of the central elevation angle (nominally zero degrees) are selected. To check that the correct sequence has been selected, a pair-wise intensity check is made on measurements on either side of the middle of the selected sequence. If the deviation from the central spectrum is too large, both readouts are discarded. Furthermore, those readouts which do not correspond to a complete band 1a readout are also discarded. The Solar Mean Reference spectrum (SMR) is calculated as the mean, after correction for the irradiance response of the instrument, of all selected detector readouts which have passed the intensity check during the solar calibration period. In addition the absolute error in the SMR is calculated. Note that an SMR spectrum can be generated for PMD data in all transfer modes. The accumulated scans must therefore be sorted on the basis of PMD transfer mode as specified in Appendix B.

This module also performs a Doppler shift correction on the SMR wavelength grid.

5.2.22.3 Variables

5.2.22.3.1 Local variables

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
k	Readout index and PMD pixel counter	i	-	t	-	
N_{meas}	Number of detector readouts in *Sun* observation mode	i	-	t	-	
N	Number of detector readouts in *Sun* observation mode passing solar elevation angle check.	i	-	t	-	
I_{pair}	Mean channel three intensity for pairs of detector readouts	d[N/2]	-	t	-	
$\langle Sun^{BU/s}\rangle$	Mean of the N_{sun} solar measurements having passed the intensity and consistency checks.	d[D,B]	BU/s	t	AX.1/–	
$\langle E_{Sun}^{BU/s}\rangle$	Error in the mean of the *Nsun* solar measurements having passed the intensity and consistency checks	d[D,B]	BU/s	t	AX.1/–	
$\overline{v_{Sat-Sun}}$	Mean relative speed of satellite and sun, for those spectra passing the intensity and consistency check	d	m/s	t	-	

5.2.22.3.2 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
δI	Intensity threshold for difference in intensity pairs	d	-	i	A2.0.1	
$e_{central}$	Central elevation angle of the Sun observation mode detector readouts	d	degree	i	A2.0.1	
δe	Maximum deviation of solar elevation from central angle	d	degree	i	A2.0.1	
t_{Nsun}	Lower limit threshold for number of detector readouts in Sun observation mode which pass the intensity check test	i	-	i	A2.0.1	
C	Speed of light.	d	m/s	i	A2.0.1	
N_{PMD}	Total number of PMD bands	w	-	i	A2.0.1	

5.2.22.3.3 Input from level 0 data stream and level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
s	Pixel number defining the start of a PMD band	$i[N_{PMD},2]$	-	i	A2.0.7 A3.0.4	MDR-1a* ISP_HEAD
l	Length in pixels of a PMD band	$i[N_{PMD},2]$	-	i	A2.0.7 A3.0.4	MDR-1a* ISP_HEAD

5.2.22.3.4 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
UTC_{Sun}	UTC date/time of valid *Sun* calibration mode measurements	d[N]	fractional days	i	A2.3	
pmd_transfer	PMD transfer mode to be used for sorting of *Sun* observation mode scans	enum[N]	-	i	A2.3	
pmd_readout	PMD readout mode	enum[N]	-	i	A2.3	
$v_{Sat\text{-}Sun}$	Relative speed of satellite and sun (negative if satellite is moving towards the sun)	d[N]	m/s	i	A2.6	
e_{meas}	Solar elevation angle of the measurement (Satellite Relative Actual CS)	d	deg	i	A2.6	
λ^{sun}	Wavelength grid of the *Sun* observation mode detector readouts	d[D,B]	nm	i	A2.15	
$Sun^{BU/s}$	Solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light and normalised to one-second integration time.	$d[D,B,N_{sun}]$	BU/s	i	A2.19	
E_{DPES}	Error in solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light, and normalised to one second integration time.	$d[D,B,N_{meas}]$	BU/s	i	A2.19	
Sun	Solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light and the irradiance response of the instrument.	$d[D,B,N_{sun}]$	photons/(s.cm^2.nm)	i	AG.18	

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
E_{Sun}	Error in solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light, and the irradiance response of the instrument.	d[D,B,N_{sun}]	photons/(s.cm^2.nm)	i	AG.18	
E_{rand}	Component of E_{Sun} attributable to shot and readout noise	d[D,B,N_{sun}]	photons/(s.cm^2.nm)	i	AG.18	
missing	Mask indicating missing mean values			i	AX.1	1 = missing 0 = not missing

5.2.22.3.5 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
Sun_{start}	Start UTC date/time of valid *Sun* calibration mode measurements	d	fractional days	o	ifc	
Sun_{end}	End UTC date/time of valid *Sun* calibration mode measurements	d	fractional days	o	ifc	
Sun_{trans}	PMD transfer mode associated with SMR measurements	enum	-	o	ifc	
Sun_{read}	PMD readout mode associated with SMR measurements	enum	-	o	ifc	
λ^{SMR}	SMR wavelength grid after Doppler correction	d[D,B]	nm	o	ifc	
SMR	Solar Mean Reference spectrum	d[D,B]	photons/(s.cm^2.nm)	o	ifc	
E_{SMR}	Absolute error in the Solar Mean Reference spectrum	d[D,B]	photons/(s.cm^2.nm)	o	ifc	
$\varepsilon_{Sun}^{BU/s}$	Relative error in the mean of the Nsun solar measurements having passed the intensity and consistency checks, before correction for the irradiance response of the instrument.	d[D,B]	-	o	ifc	
N_{sun}	Number of detector readouts in *Sun* observation mode which pass the intensity check test.	w		o	ifc	
F_{Nsun}	Flag indicating that number of detector readouts in *Sun* observation mode passing the intensity check test is too low.	bool	-	o	ifc	1 = number of spectra too low 0 = number of spectra sufficient
F_{Sun}^{miss}	Flag indicating that no SMR was generated due to missing mean Sun mode measurements per channel.	bool[B]	-	i/o	ifc	1 = no SMR for given channel 0 = not missing

5.2.22.4 Algorithm

5.2.22.4.1 Sort Scans from Sun Observation Mode (A2.20.1)

All scans accumulated in one Sun observation mode period are sorted on the basis of PMD transfer (*pmd_transfer*) mode. The following calculation of SMR applies to each sorted group. In thecae that *pmd_transfer = raw* simulated SMR PMD band data are created from the measured SMR PMD raw data and provided in the final product. Note also that the SMR is calculated per channel. Main channel bands need only be separated prior to the calculation of a mean *Sun* spectrum. Note that the spectral calibration can be assumed to be constant during one *Sun* calibration mode period.

5.2.22.4.2 Calculate SMR and Absolute Error (A2.20.2)

In the following steps, a subset of readouts fulfilling certain conditions will be selected from the sequence readouts in sun mode. This is done to ensure proper illumination conditions for the selected readouts. It is important to note that the resulting series of readouts has to be continuous (in time), i.e., readouts shall only be removed from the beginning and the end of the series, never from the middle.

- For $k = 1 \ldots N_{meas}$ then exclude detector readout k from processing of the SMR if $|e_{meas,k} - e_{central}| > \delta e$ yielding N useful detector readouts from *Sun* observation mode.
- Intensity pairs are calculated from the total intensity in channel 3 as:

$$I_{pair,k} = \frac{1}{2} \cdot \left(\sum_{i=0}^{D_j - 1} Sun_{k,i3}^{BU/s} + \sum_{i=0}^{D_j - 1} Sun_{(N-k),i3}^{BU/s} \right)$$ *Equation 139*

- Pairs are discarded for which:

$$\left| \frac{I_{pair,k}}{I_{pair,N/2}} - 1 \right| > \delta I$$ *Equation 140*

  This is done starting from the central pair $k = N/2$, and going outwards until the first pair fulfils (140). This pair and all readouts before the first readout in the pair and after the last one are discarded.

- Those band readouts which have passed the intensity check but for which no complete corresponding band 1a readout is available are also discarded. Note that this implies starting from the *second* valid band 1a readout during the valid readouts of the bands with shorter integration times, because the *first* valid band 1a readout has started at a time where the readouts of the bands with shorter integration times were not yet valid

- The remaining N_{sun} spectra which have passed the intensity and correspondence check are corrected for the irradiance response of the instrument using Apply Irradiance Response (AG.18) yielding *Sun*, E_{sun} and E_{rand} .
- The SMR and the absolute error in the SMR, taking into account the reduction of random noise by averaging, are calculated as the mean of the N_{sun} spectra using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1).
- In the case that there are detector pixels with no valid readouts in any channel as indicated by *missing*, no SMR is generated for that channel.
- If *pmd_transfer = raw* create virtual SMR PMD band measurements for $i = 1...N_{PMD}$ and $j = 7...8$ as follows:

$$SMR_{ij} = \frac{1}{l_{ij}} \cdot \sum_{k = s_{ij}}^{s_{ij} + l_{ij} - 1} SMR_{kj}$$ *Equation 141*

- Additionally, the absolute error in the virtual SMR PMD bands is calculated as follows:

$$E_{SMR,\,ij} = \sqrt{\sum_{k = s_{ij}}^{s_{ij} + l_{ij} - 1} (E_{SMR,\,kj})^2}$$ *Equation 142*

- The wavelengths associated with the virtual SMR PMD bands are calculated from λ^{Sun} as described in Apply Spectral Calibration (AG.14).
- Note that when *pmd_transfer = raw* the first 745 pixels are unused and are therefore available to store the simulated SMR PMD band measurements.

5.2.22.4.3 *Calculate the Relative Error in the Mean Spectrum (BU/s (A2.20.3)*

- The mean $\overline{\langle Sun^{BU/s} \rangle}$ and the mean absolute error $\overline{\langle E^{BU/s}_{Sun} \rangle}$ of the N_{sun} spectra having passed the intensity and correspondence checks are calculated from $Sun^{BU/s}$ and E_{DPES} using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1). In this case the reduction of random noise by averaging is not taken into account as this is expected to be insignificant with respect to the error in the MMEs.
- Any detector pixels for which there are no valid readouts, as indicated by *missing*, are assigned mean values which are equal to a linear interpolation between the nearest valid neighbouring values calculated using Linear Interpolation (AX.2). In the case that an entire channel is missing, nothing is calculated for that channel.
- The mean relative error in the N_{sun} spectra, before correction for the irradiance response of the instrument, is calculated for $i = 0...D_j - 1$, $j = 1...B$ as:

$$\varepsilon_{Sun,\,ij}^{BU/s} = \frac{\langle E_{Sun,\,ij}^{BU/s}\rangle}{\langle Sun_{ij}^{BU/s}\rangle} \qquad \text{Equation 143}$$

Note: This quantity is used in the estimation of the absolute error in the sun-normalised radiance in Apply Irradiance Response (A3.12).

5.2.22.4.4 Correct Doppler Shift (A2.20.4)

Calculate the mean relative speed of satellite and sun for those solar spectra passing the intensity and correspondence check test as follows:

$$\overline{v_{\text{Sat-Sun}}} = \frac{1}{N_{sun}} \sum_{k=1}^{N_{sun}} v_{\text{Sat-Sun},\,k} \qquad \text{Equation 144}$$

Correct the SMR wavelength grid for the Doppler shift in the measured solar spectra, using module Correct Doppler Shift (AG.19) with c, $\overline{v_{\text{Sat-Sun}}}$ and λ^{Sun} on input. This returns the Doppler-corrected wavelength grid λ^{SMR}.

5.2.22.4.5 Calculate PCDs From SMR

Assuming F_{Nsun} has been initialised to zero then if:

$$N_{sun} < t_{Nsun} \qquad \text{Equation 145}$$

set

$$F_{Nsun} = 1 \qquad \text{Equation 146}$$

Furthermore, assuming F_{Sun}^{miss} has been initialised to zero, then if there are missing mean values in channel j and therefore no SMR calculated set $F_{Sun,j}^{miss} = 2$.

5.2.23 Determine Stokes Fractions (A2.21)

Instrument Modes		Instrument Data	
Earth (PMD only)	√	PMD	√
Dark		FPA	
Sun		Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

Spline Interpolation (AX.3)

Data Granule

One Scan, with access to the previous scan.

5.2.23.1 Objectives

Calculate Stokes fractions from measurement geometry and preprocessed PMD measurements.

5.2.23.2 Description

GOME-2 is a polarisation-sensitive instrument. The measured signals are determined by the total intensity and the polarisation state of the incoming light. The 0 to 1b processor has the task to derive the total intensity from the measured signals. Therefore the polarisation state of the incoming light has to be characterised. This will be done by this module, utilising the measurements of the PMD channels and observation geometry. The module Apply Polarisation Correction (A3.10)will later on use this information to correct the signals measured in the main channels for the polarisation sensitivity of the instrument. Additionally, if *pmd_transfer* = *raw* and *pmd_readout* = *nominal* or *solar* the Stokes fractions are calculated at full PMD spectral resolution and reported in the product for instrument monitoring and scientific use. Note that in the latter case the Stokes fractions generated are not used for the main channel polarisation correction.

The algorithm uses the representation introduced in Appendix E.2 where the intensity and polarisation state of the light is expressed in terms of a Stokes vector $\boldsymbol{I} = (I,Q,U,V) \equiv \mathrm{I}\,(1,q,u,v)$. The Stokes elements I,Q,U,V have the dimension of an intensity. The Stokes fractions $q \equiv Q/I$, $u \equiv U/I, v \equiv V/I$ are dimensionless and assume values between –1 and +1. The instrument transmission for polarised light is expressed in terms of Müller matrices **M**, so that $\boldsymbol{S} = \mathbf{M}\,\boldsymbol{I}$, where $\boldsymbol{I}$ describes the incoming radiance and $\boldsymbol{S}$ the polarised intensity at the detector. In the following, we are only concerned with the first component (total intensity) of $\boldsymbol{S}$ which we call S. Therefore, only the first row of the Muller matrices is needed, where we abbreviate elements M^{11}, M^{12}, M^{13}, as M^1, M^2, M^3. By definition, Stokes fractions and Muller matrix elements depend on the choice of a reference frame. For this module, the following will be assumed.

- The reference coordinate frame for the Stokes vectors is the local meridian plane (XZ plane of the Satellite Relative Actual Reference Coordinate System). See Appendix C for details.

- The fraction of circularly-polarised light of the total incoming light can be neglected: $V = 0$. Only linearly-polarised light is considered.

The measured signal can then (for all channels, main FPAs and PMDs) be expressed as follows:

$$S = M^1 I + M^2 Q + M^3 U = M^1 I(1 + \mu^2 q + \mu^3 u) \qquad \text{Equation 147}$$

where $\mu^2 \equiv M^2/M^1$, $\mu^3 \equiv M^3/M^1$, $q \equiv Q/I$, $u \equiv U/I$ as usual, and all quantities are wave-length dependent. Stokes fractions *q* will be derived by this module from the PMD measurements. This will be done on the wavelength grid given by the PMD bands (the wavelength assignment itself is irrelevant at this stage). Single-scattering Stokes fractions *u* will also be derived by this module, using observation geometry alone (i.e., no spectral measurements). The Müller matrix elements M^1, μ^2, μ^3 characterising the instrument have been derived from the calibration key data in module Preprocess Müller Matrix Elements (A2.1). The module Apply Polarisation Correction (A3.10) will later on interpolate the Stokes fractions *q* to the full wavelength grid of the main channels and use Equation 147 to derive the incoming intensity *I* from the measured signal *S*. For *u*, the single-scattering value calculated below will be used, assuming its wavelength dependence can be neglected.

PMD s is sensitive to light polarised perpendicular to the instrument slit (parallel to the reference plane, $\mu_s^2 \approx +1$), PMD p is sensitive to light polarised parallel to the instrument slit (perpendicular to the reference plane, $\mu_s^2 \approx 1$). This allows Stokes fractions to be derived solely from the ratios of PMD s and PMD p signals. Main channel signals are not involved.

Note: This is a fundamental advantage compared to the situation for GOME-1 and SCIAMACHY. Main channel signals are, however, needed for the PMD wavelength calibration (and PMD stray light correction).

To be able to ratio signals from PMD s and PMD p a further assumption has to be made, it is assumed that PMD s and PMD p are sufficiently well co-registered in wavelength that the interpolation does not introduce a significant error into the Stokes fractions derived from their ratios in this module.

For use in the main channel polarization algorithm, Stokes fractions will be derived per PMD band, thereby covering approximately the wavelength range of main channels 2 to 4. A theoretical value based on the assumption of Rayleigh single-scattering allows extension of these values for the UV beyond the nominal range of the PMD measurements. Therefore, this module consists of two parts:

1. Calculate Rayleigh single-scattering Stokes fractions. For wavelengths below approximately 300 nm the strong absorption by ozone prevents the solar radiation from penetrating deeply into the earth’s atmosphere. Scattering typically occurs at large heights so that scattering by molecules is the dominating scattering process. In this case, the Stokes fraction of the incoming light can be readily calculated from theory. It depends only on the measurement geometry (solar and line-of-sight angles). It is performed on the time grid of the shortest effective integration time in the main channels (187.5 ms).
2. Calculate Stokes fractions from PMD measurements. With ozone absorptions decreasing towards higher wavelengths, the radiation reaches lower layers of the atmosphere and ultimately the surface. Multiple Rayleigh scattering, scattering at particles and reflection from the ground change the polarisation state of the radiation, in general depolarising the incoming signal compared to the Rayleigh single-scattering case. Stokes fractions are calculated for each of the 15 PMD bands and (i) for each PMD readout (signal level permitting) and (ii) for PMD

readouts averaged into 187.5 ms bins. In the case that *pmd_transfer = raw* the number of spectral points is 256 and the number of readouts is 16 (corresponding to a nominal integration time of 0.375 s).

For the single-scattering case, the Stokes fractions will be calculated from the total degree of linear polarisation *P* and the angle χ between the polarisation plane (containing the line-of-sight and the polarisation direction) and the reference plane (the local meridian plane, containing the line-of-sight and the nadir direction). These quantities are related to the Stokes fraction *q*, *u* according to this:

$$q = P\cos 2\chi \quad \text{Equation 148}$$

$$u = P\sin 2\chi \quad \text{Equation 149}$$

P does not depend on the choice of reference plane while χ, and therefore *q* and *u* obviously do.

Note: For completeness, the relations between Stokes fractions *q*, *u* on one side and degree of linear polarisation *P* and polarisation angle χ on the other side are given here: $P = \sqrt{q^2 + u^2}$ and $\chi = \frac{1}{2}\mathrm{atan}\frac{u}{q}$. For GOME-1, the fractional polarisation p parallel to the entrance slit direction (perpendicular to our reference plane) was commonly used $p = \frac{1}{2}(1 - q)$.

PMD measurements on input have to be dark signal and stray light corrected. PMD data to be used for the main channel polarisation correction is assumed to be transferred in band mode. If this is not the case, it is indicated by a flag set in Determine Observation Mode and Viewing Angles (A2.3) the calculations are not carried out.

Stokes fractions for light backscattered from the earth's atmosphere are expected to be between zero (unpolarised) and the Stokes fraction for single-scattering. This is because additional scattering, e.g., in clouds, always depolarises the light. Stokes fractions calculated for the main channel polarisation correction will be checked and flagged "bad" if they do not meet this expectation. This check assumes that the polarisation angle is not wavelength-dependent. This assumption does not hold for PMD bands below a certain wavelength (typically 600 nm) with a low singles-scattering degree of polarisation which are, therefore, not checked.

PMD measurements are also used to derive an indicator for the scene variability within a main channel readout. This is useful as a quality indicator: the higher the intensity variation within a main channel readout, the higher are the systematic errors introduced by spatial aliasing, both directly into the measured FPA signals (because different FPA detector pixels observe different scenes), and indirectly via the polarisation correction (because PMD and FPA detector pixels observe different scenes).

5.2.23.3 Variables

5.2.23.3.1 Indices

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
i	PMD band index	i	-	t	-	$0 \ldots N_{PMD}-1$
j	PMD ban	i	-	t	-	$0 \ldots R_{PMD}-1$
j_1	First PMD readout index for PMDsum	i	-	t	-	Negative values refer to previous scan, see text.
j_2	Last PMD readout index for PMDsum	i	-	t	-	Negative values refer to previous scan, see text.
l	High resolution viewing-angle fixed grid index	i	-	t	-	$0 \ldots N_{\psi h}-1$
k	Index number of current scan mirror readout within scan (including extra entry at the end)	i	-	t	-	$0 \ldots R_{\psi}$
m	Index of Stokes fraction set for main channel correction	i	-	t	-	$0 \ldots 3$
n	Index number of current 187.5 ms ground pixel within scan	i	-	t	-	$0 \ldots R_{FPA}-1$. Read-out 0 is the first readout in the first data packet of the scan.

5.2.23.3.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
N_ψ	Number of viewing angles for which calibration key data are measured	w	-	i	A2.0.4	
ψ	Viewing angles for which calibration key data are measured	$d[N_\psi]$	degree	i	A2.0.4	
S^s_{req}	Minimum required PMD-s signal	d	BU	i	A2.0.1	
S^p_{req}	Minimum required PMD-p signal	d	BU	i	A2.0.1	
M_{SSP}	Number of zenith angle / wave-length pairs for single-scattering parameterisation	i	-	i	A2.0.1	
$\theta_{Sun,SSP}$	Solar zenith angle for single-scattering parameterisation	$d[M_{SSP}]$	degrees	i	A2.0.1	
λ_{SSP}	Wavelength of single-scattering value corresponding to θSun,SSP	$d[M_{SSP}]$	nm	i	A2.0.1	
$P_{\mathrm{SS,min,BadStokes}}$	Minimum single-scattering degree of polarisation for Stokes fractions to be checked	d	-	i	A2.0.1	
$\lambda_{\mathrm{min,Bad\text{-}Stokes}}$	Minimum PMD band wavelength for Stokes fractions to be checked	d	nm	i	A2.0.1	
δq	Tolerance for Stokes fraction check	d	-	i	A2.0.1	
Δ_{depol}	Depolarisation parameter for Rayleigh scattering	d	-	i	A2.0.1	
i_{Scene}	Index of PMD band from which scene variability is derived (zero-based)	d	-	i	A2.0.1	
$q_{\mathrm{SS,\ min}}$	Lower threshold for single-scattering Stokes fraction q_{SS} to avoid singularity in $u_{\mathrm{SS}}/q_{\mathrm{SS}}$	d	-	i	A2.0.1	
$\cos(2\chi)_{SS,\ min}$	Minimum cosine of two times the polarisation angle for Rayleigh scattering below which q = 0	$d[R_{FPA}]$	-	i	A2.0.1	*0.08*
m_{qc}	PMD signal ratio tolerance for accepting correction signals for special geometry readouts	d	-	i	A2.0.1	*0.1*
N^{qc}	Minimum number of PMD radio-metric response ratio corrections accumulated until writing of mean values to COR file for all high resolution viewing angles Ψ^h and MME wavelengths	d	-	i	A2.0.1	*9*
$\Delta^{t,,qc}$	Maximum number of days for accumulation of PMD radiometric response ratio corrections	d	-	i	A2.0.1	*29*
$\Delta^{h,qc}$	Maximum difference between actual viewing angle for PMD read-out *j* and nearest neighbour gridpoint *h* on high-resolution Ψ^h viewing angle grid	d	-	i	A2.0.1	*0.1*

5.2.23.3.3 Input from correction dataset

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
$N_{\psi h}$	Number of angles for which the high resolution viewing-angle grid is specified.	d	-	i	A2.0.5	
ψ^h	High resolution viewing-angle grid	d[$N_{\psi h}$]	-	i	A2.0.5	
$\overline{M^{\eta D}_{\psi^h}}$	Default correction for PMD radiometric response ratio from special geometries per MME wavelength and high resolution viewing angle.	d[D,$N_{\psi h}$]	-	i	A2.0.5	*Note that in these cases D refers to the number of points in the MME wave-length grid*
$\overline{M^{\eta}_{\psi^h}}$	Correction for PMD radiometric response ratio from special geometries per high-resolution viewing angle and MME wavelength.	d[D,$N_{\psi h}$]	-	i	A2.0.5	*Note that in these cases D refers to the number of points in the MME wave-length grid*

5.2.23.3.4 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
λ^{MME}	Wavelength grid on which the Müller Matrix Elements are calculated.	d[D,B]	nm	i	A2.1	
$M^1(s/p)$	Radiometric response ratio of PMD-s/PMD-p as a function of viewing angle	d[D, $N_{\psi f}$]	-	i	A2.1	
μ^2	Ratio of MMEs M^2 to M^1 describing the polarisation sensitivity of the instrument with respect to the QStokes component (s/p polarisation). Derived from key data parameter.	d[D,B, $N_{\psi f}$]	-	i	A2.1	
μ^3	Ratio of MMEs M^3 to $M1$ describing the polarisation sensitivity of the instrument with respect to the UStokes component (+/–45° polarisation). Derived from keydata parameter ξ.	d[D,B, $N_{\psi f}$]	-	o	A2.2	

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
IT	Integration time per band	i [N_{PMD}]	s	i	A2.3	
pmd_transfer	PMD transfer mode	enum[N]	-	i	A2.6	
Θ	Scattering angle, h_0, EFG (topocentric CS)	d[R_{FPA},3]	degree	i	A2.6	
φ_{Sat}	Satellite azimuth, h_0, EFG (topocentric CS)	d[R_{FPA},3]	degree	i	A2.6	Only the angles for ground pixel centre (point F) will be used for the FPA grid. Points EFG are used for the PMD grid Stokes fractions calculation.
φ_{Sun}	Solar azimuth, h_0, EFG (topocentric CS)	d[R_{FPA},3]	deg	i	A2.6	
θ_{Sat}	Satellite zenith, h_0, EFG (topocentric CS)	d[R_{FPA},3]	deg	i	A2.6	
θ_{Sun}	Solar zenith, h_0, EFG(topocentric CS)	d[R_{FPA},3]	deg	i	A2.6	
ψ	Scanner viewing angle with additional element at end of scan	d[R_{ψ}+1]	deg	i	A2.6	
S^S	PMD s signals, dark signal and stray light corrected, and normalised to one-second integration time.	d[N_{PMD},R_{PMD}]	BU/s	i	AG.17	
S^p	PMD p signals, dark signal and stray light corrected, and normalised to an integration time of one second.	d[N_{PMD},R_{PMD}]	BU/s	i	AG.17	
λ	Wavelength grid associated with PMD band readouts.	d[N_{PMD}]	nm	i	A2.14/A2.23.1	**MDR-1*-Earthshine** *POL_MWL_POL* *POL_M_PWL_POL*

5.2.23.3.5 Local variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
$S^{s,MME}$	PMD s signals, dark signal and stray light-corrected, and normalised to one-second integration time and interpolated onto the MME wave-length grid.	$d[D,R_{PMD}]$	BU/s	i	AG.17	*Note that in these cases D refers to the number of points in the MME wavelength grid*
$S^{p,MME}$	PMD p signals, dark signal and stray light corrected, and normalised to an integration time of one second and interpolated onto the MME wavelength grid.	$d[D,R_{PMD}]$	BU/s	i	AG.17	*Note that in these cases D refers to the number of points in the MME wavelength grid*
$M^1_{(s/p),\Psi}$	Radiometric response ratio of PMDs and PMD p interpolated to a viewing angle Ψ (which will be either Ψ_i or $\overline{\Psi}$ below).	d[D]	-	t		
$\mu^2_{p,\Psi}$	Ratio of MMEs M^2 to M^1 that describe the polarisation sensitivity of the instrument for PMD p band interpolated to a viewing angle Ψ.	d[D]	-	t		
$\mu^2_{s,\Psi}$	Ratio of MMEs M^2 to M^1 that describe the polarisation sensitivity of the instrument for PMD s band interpolated to a viewing angle Ψ.	d[D]	-	t		
$\mu^3_{p,\Psi}$	Ratio of MMEs M^3 to M^1 that describe the polarisation sensitivity of the instrument for PMD p band interpolated to a viewing angle Ψ.	d[D]	-	t		
$\mu^3_{s,\Psi}$	Ratio of MMEs M^3 to M^1 that describe the polarisation sensitivity of the instrument for PMD s band interpolated to a viewing angle Ψ.	d[D]	-	t		
Ψ	Viewing angles corresponding to individual PMD readouts, i.e., on 23.4 ms grid. One extra element at the end for convenience.	$d[R_{PMD}+1]$	degree	t		A capital Ψ is used to distinguish the variable from the viewing angle ψ on the 93.75 ms grid.

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
$\overline{\Psi}$	Averaged viewing angle corresponding to an average (in time) of PMD readouts.	d	degree	t	-	
$\overline{S}^{s,MME}$	Time averaged PMD s signals.	d	BU/s	t	-	
$S^{p,MME}$	Time averaged PMD p signals.	d	BU/s	t	-	
α	Temporary variable to simplify calculation of polarisation angle.	d	-	t	-	
$\overline{S}_{Scene}$	Average over 8 PMD readouts (sum over both PMD detectors).	d	BU/s	t	-	
M^{qc}	Actual correction for PMD radiometric response ratio for special geometries on the MME wave-length grid and per PMD readout.	d[D,R_{PMD}]	-	t	-	
$M^{qc}_{\Psi^h}$	Accumulated correction for PMD radiometric response ratio from special geometries on the MME wavelength grid and per high resolution viewing angle.	i[D,$N_{\psi h}$]	-	t	-	*Stored in CTX file*
$N^{c}_{\Psi^h}$	Number of PMD radiometic response ratio corrections accumulated per MME wavelength and high resolution viewing angle.	i[D,$N_{\psi h}$]	-	t	-	*Stored in CTX file*
$\overline{N^{c}_{\Psi^h}}$	Number of PMD radiometric response ratio corrections accumulated per high resolution viewing angle and averaged over wave-length.	i[D,$N_{\psi h}$]	-	t	-	
$\overline{M^{qc}_{\Psi}}$	Correction to the PMD radiometric response ratio interpolated to a viewing angle Ψ.	[D]	-	t	-	
φ^{Ψ}	Generic variable used for Θ^{Ψ}, φ^{Ψ}_{Sat}, φ^{Ψ}_{Sun}, θ^{Ψ}_{Sat}, and θ^{Ψ}_{Sun} on the scanner angle grid.	d[R_{ψ}+1]	degree	t	-	
Θ^{Ψ}	Scattering angle, h_0, on the scanner angle grid (topocentric CS).	d[R_{ψ}+1]	degree	t	-	
φ^{Ψ}_{Sat}	Satellite azimuth, h_0, on the scanner angle grid (topocentric CS).	d[R_{ψ}+1]	degree	t	-	
φ^{Ψ}_{Sun}	Solar azimuth, h_0, on the scanner-angle grid (topocentric CS) .	d[R_{ψ}+1]	degree	t	-	
θ^{Ψ}_{Sat}	Satellite zenith, h_0, on the scanner angle grid (topocentric CS).	d[R_{ψ}+1]	degree	t	-	
θ^{Ψ}_{Sun}	Solar zenith, h_0, on the scanner angle grid (topocentric CS).	d[R_{ψ}+1]	degree	t	-	
P^{Ψ}_{SS}	Degree of linear polarisation for Rayleigh single-scattering on the scanner angle grid.	d[R_{ψ}+1]	-	t	-	

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
χ_{ss}^{Ψ}	Polarisation angle for Rayleigh single-scattering on the scanner angle grid	$d[R_\psi+1]$	deg	t		
$\cos(2\chi_{ss}^{\Psi})$	Cosine of two times the polarisation angle for Rayleigh scattering on the scanner angle grid.	$d[R_\psi+1]$	-	t		
q_{ss}^{Ψ}	Stokes fractions (0°/90°) for Rayleigh single-scattering on scanner angle grid	$d[R_\psi+1]$	-	t		
u_{ss}^{Ψ}	Stokes fractions (-45°/45°) for Rayleigh single-scattering on scanner angle grid	$d[R_\psi+1]$	-	t		
$P_{ss,\Psi}$	Degree of linear polarisation for Rayleigh single-scattering on the viewing angle grid for PMDs	$d[R_{PMD}]$	-	t		
$\chi_{ss,\Psi}$	Polarisation angle for Rayleigh single-scattering on the viewing angle grid for PMDs	$d[R_{PMD}]$	degree	t		
$\cos(2\chi_{SS,\Psi})$	Cosine of two times the polarisation angle for Rayleigh scattering on viewing angle grid for PMDs	$d[R_{PMD}]$	-	t		
q_{ss,Ψ_j}	Stokes fractions (0°/90°) for Rayleigh single-scattering per PMD viewing angle	$d[R_{PMD}]$	-	t		
u_{ss,Ψ_j}	Stokes fractions (-45°/45°) for Rayleigh single-scattering per PMD viewing angle	$d[R_{PMD}]$	-	t		
q^{MME}	Stokes fractions per PMD readout on the MME wavelength grid	$d[D, R_{PMD}]$	-	t		
$q^{Sun,\ MME}$	Sun Stokes fractions per PMD read-out on the MME wavelength grid	$d[D, R_{PMD}]$	-	t		
$\overline{q^{MME}}$	Stokes fractions per main channel readout (187.5 ms) on the MME wavelength grid for main channel polarisation correction	$d[D, 4, R_{FPA}]$	-	t		

5.2.23.3.6 Global PCDs accumulated per product

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
$N_{MissStokes}$	Number of scans with missing Stokes fractions.	w[N_{PMD}]	-	g	A2.22	
$N_{BadStokes}$	Number of scans with bad Stokes fractions.	w[N_{PMD}]	-	g	A2.22	

5.2.23.3.7 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
P_{SS}	Degree of linear polarisation for Rayleigh single-scattering	d[R_{FPA}]	-	o	A2.23.1	**MDR-1*-Earthshine** POL_SSP_POL_SS
χ_{SS}	Polarisation angle for Rayleigh single-scattering	d[R_{FPA}]	deg	o	A2.23.1	**MDR-1*-Earthshine** POL_SSCHI_POL_SS
q_{SS}	Stokes fractions (0°/90°) for Rayleigh single-scattering	d[R_{FPA}]	-	o	A2.23.1	**MDR-1*-Earthshine** POL_SSQ_POL_SS
u_{SS}	Stokes fractions (–45°/+45°) for Rayleigh single-scattering	d[R_{FPA}]	-	o	A2.23.1	**MDR-1*-Earthshine** POL_SSU_POL_SS
λ_{SS}	Single-scattering wavelength	d[R_{FPA}]	nm	i/o	A2.14/A2.23.1	**MDR-1*-Earthshine** POL_SSWL_POL_SS
q	Stokes fractions per PMD band and PMD readout	d[N_{PMD}, R_{PMD}]	-	o	A2.23.1	**MDR-1*-Earthshine** POL_M_PQ_POLPOL_M_SW
q^{Sun}	Sun Stokes fractions per PMD band and PMD readout.	d[N_{PMD}, R_{PMD}]	-	o	A4.2.17	*To be written to the MON file.*
$\overline{q}$	Stokes fractions per PMD band and main channel readout (187.5 ms) for main channel polarisation correction.	d[N_{PMD}, 4,R_{FPA}]	-	o	A2.23.1	**MDR-1*-Earthshine** POL_MQ_POL
$F_{MissStokes}$	Flag indicating missing Stokes fractions *q* in scan (per PMD band).Stokes fractions may be missing because of too low PMD signals. Stokes fractions missing due to PMD reset (occurring in every scan) are not flagged. Missing Stokes fractions *q* are not flagged here, but in the overall MDR degradation flag.	bool[N_{PMD}]	-	o	A2.23.1	**MDR-1*-Earthshine** PCD_EARTHF_MISS_STOKES 1 = some missing 0 = all present

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
$F_{\mathrm{BadStokes}}$	Flag indicating bad Stokes fractions in scan. Bad Stokes fractions are those which have been calculated but seem suspicious compared tithe expectations.	bool[N_{PMD},R_{FPA}]	-	o	A2.23.1	**MDR-1*-Earthshine** PCD_EARTH F_BAD_STOKES 1 = bad 0 = OK or not checked
σ_{Scene}	Normalised standard deviation of 8 PMD readouts, indicating scene variability within a 187.5 ms ground pixel.	d[R_{FPA}]	-	o	A2.23.1	**MDR-1*-Earthshine** PCD_EARTHSIGMA_SCENE
$\overline{M^{1e}_{\psi^h}}$	Updated correction for PMD radiometric response ratio from special geometries per MME wavelength and high resolution viewing angle.	d[D,$N_{\psi h}$]	-	o	corr	*Stored in the COR file*
σ^{M1e}_{ψ}	Standard deviation derived from calculation of the following: $\overline{M^{1e}_{(i),\psi^h}}$ per high resolution viewing angle and MME wavelength.	d[D,$N_{\psi h}$]	-	o	corr	*Stored in the COR file*
$M^{1e}_{(s/p)}$	Corrected radiometric response ratio of PMD-s/PMD-p as a function of viewing angle.	d[D,$N_{\psi f}$]	-	i	A2.1	

5.2.23.4 Algorithm

If *pmd_transfer = band* or *pmd_transfer = mixed* the following calculations are carried out for those data packets transferred in band mode, otherwise if *pmd_transfer = raw* and *pmd_readout =nominal* or *solar* the following calculations are carried out at full PMD spectral resolution for scientific use.

5.2.23.4.1 Calculate Rayleigh Single-Scattering Stokes Fractions for FPAS (A2.21.2)

Loop information: The following calculations will be performed for all 187.5 ms subpixels of a scan (32 times), i.e., for $n = 0 \ldots R_{FPA}-1$.

Degree of polarisation P and polarisation angle χ for single-scattering by molecules depend on the measurement geometry only.

From the scattering angle Θ_n, provided by the module Calculate Geolocation for Fixed Grid (A2.6) for the centre point (F) of a 187.5 ms ground pixel, calculate $\cos^2\Theta_n$.

For the very special case of $\cos^2\Theta_n = 1$ (direct forward or backward scattering), we set $P_{SS},n = 0$, $\chi_{SS,n} = 0$, $q_{SS,n} = 0$, $u_{SS,n} = 0$ and are finished. Otherwise these quantities are calculated as follows.

The single-scattering degree of polarisation PSS depends on the scattering angle Θ and the depolarisation parameter Δ_{depol} only:

$$P_{SS,n} = \frac{1 - \cos^2\Theta_n}{1 + \Delta_{depol} + \cos^2\Theta_n}$$ *Equation 150*

Then, calculate

$$\alpha = \mathrm{acos}((\sin\theta_{Sat,nF} \cdot \cos\theta_{Sun,nF} + \sin\theta_{Sun,nF} \cdot \cos\theta_{Sat,nF} \cdot \cos(\varphi_{Sat,nF} - (\varphi_{Sun,nF} + 180°)))/\sin\Theta)$$ *Equation 151*

where $\sin\Theta = \sqrt{1 - (\cos\Theta)^2}$

Next, the single-scattering direction of polarisation is calculated as follows:

$$\chi_{ss} = 90 - \alpha \text{ if } \sin(\varphi_{Sat,nF} - (\varphi_{Sun,nF} + 180°)) > 0 \text{ or}$$ *Equation 152*

$$\chi_{ss} = 90 + \alpha \text{ if } \sin(\varphi_{Sat,nF} - (\varphi_{Sun,nF} + 180°)) \leq 0 \text{ and where}$$ *Equation 153*

$$\chi_{ss} = \chi_{ss} - 180° \text{ if } \chi_{ss} = \chi_{ss} > 180° \text{ and}$$ *Equation 154*

$$\chi_{ss} = \chi_{ss} + 180° \text{ if } \chi_{ss} = \chi_{ss} \leq -180°$$ *Equation 155*

The single-scattering Stokes fractions q_{SS} and u_{SS} are then calculated from P_{SS}, $\cos(2\chi_{SS})$, and $\sin(2\chi_{SS})$ as follows:

$$q_{SS,n} = P_{SS,n} \cdot \cos(2\chi_{SS,n})$$ *Equation 156*

$$u_{SS,n} = P_{SS,n} \cdot \sin(2\chi_{SS,n})$$ *Equation 157*

Assign a wavelength $\lambda_{SS,n}$ to the single-scattering Stokes fraction $q_{SS,n}$: Starting from the ($\theta_{Sun,SSP}$, λ_{SSP}) pairs from the initialisation dataset, determine the single-scattering wavelength $\lambda_{SS,n}$ corresponding to the solar zenith angle $\theta_{Sun,F}$ using Spline Interpolation (AX.3).

End of loop.

Note: For the correction of main channel readout *n*, single-scattering Stokes fraction $n - 1$ will have to be used. See Apply Polarisation Correction (A3.10).

5.2.23.4.2 Calculate Rayleigh Single-Scattering Stokes Fractions for PMDs (A2.21.3)

All angles E, F, and G of φ_{Sat}, θ_{Sat}, φ_{Sun}, and θ_{Sun} are used to reconstruct a smoothed angle grid, averaging over the region δ_{Ψ} (see Figure 18) of overlap between adjacent ground pixels, for the $R_{\Psi} + 1$ scanner angle positions. See also Figure 23.

Loop information:

Repeat the following calculations for all of Θ, φSat, θ_{Sat}, φ_{Sun}, and θ_{Sun} to yield Θ^{Ψ}, φ^{Ψ}_{Sat}, θ^{Ψ}_{Sat}, φ^{Ψ}_{Sun}, and θ^{Ψ}_{Sun}. The generic variables φ and φ^{Ψ} are used in the subsequent equations.
For $n = 0 \ldots R_{FPA} - 1$ then:

Using angles for point F and for those scanner angle indices *k* where $k = 2n + 1$ set:

$$\varphi^{\Psi}_{k} = \varphi^{\Psi}_{n}$$ *Equation 158*

Using angle for points E and G first the forward and backward scans must be separated.

For the forward scan positions where $n = 0 \ldots ¾ \times R_{FPA} - 2$ and for those scanner angle indices *k* where $k = 2n + 2$ calculate as follows:

$$\text{If } |\varphi_{n,G} - \varphi_{n+1,E}| < 0.5 \text{ then } \varphi^{\Psi}_{k} = 0.5(\varphi_{n,G} + \varphi_{n+1,E})$$

$$\text{If } |\varphi_{n,G} - \varphi_{n+1,E}| \geq 0.5 \text{ then } \varphi^{\Psi}_{k} = \varphi_{n,G}$$

For the backward scan positions where $n = ¾ \times R_{FPA} \ldots R_{FPA} - 2$ and for those scanner angle indices k where $k = 2n + 2$ calculate with the order of points E and G reversed as follows.

$$\text{If } |\varphi_{n,E} - \varphi_{n+1,G}| < 0.5 \text{ then } \varphi^{\Psi}_{k} = 0.5(\varphi_{n,E} + \varphi_{n+G})$$

$$\text{If } |\varphi_{n,E} - \varphi_{n+1,G}| \geq 0.5 \text{ then } \varphi^{\Psi}_{k} = \varphi_{n,E}$$

For the special case of point G at the transition between forward and backward scans where $n = ¾ \times R_{FPA} - 1$ calculate as follows:

$$\varphi_k^{\Psi} = \varphi_{n+1,G}$$

Finally, the start and end point corresponding to $k = 0$ and $k = R\psi + 1$ are set to:

$$\varphi_0^{\Psi} = \varphi_{0,E} \text{ and}$$

$$\varphi_{R_\psi+1}^{\Psi} = \varphi_{R_\psi+1,E}$$

End loop.

Now P_{ss}^{Ψ}, $\cos(2\chi_{ss}^{\Psi})$, $\sin(2\chi_{ss}^{\Psi})$, χ_{ss}^{Ψ}, q_{ss}^{Ψ}, and u_{ss}^{Ψ} are calculated as per the description in Calculate Rayleigh Single-scattering Stokes Fractions for FPAs (A2.21.2) but replacing , Θ, φ_{Sat}, θ_{Sat}, φ_{Sun}, and θ_{Sun} with Θ^{Ψ}, φ_{Sat}^{Ψ}, θ_{Sat}^{Ψ}, φ_{Sun}^{Ψ}, and θ_{Sun}^{Ψ}.

5.2.23.4.3 Calculate Stokes Fractions from PMD Measurements (A2.21.4)

5.2.23.4.3.1 Determine viewing angle and single-scattering Stokes fraction grid for individual PMD readouts

We need to prepare the calculation of Stokes fractions for individual PMD readouts. For this step, viewing angles and single-scattering Stokes fractions are needed for each PMD readout, i.e., every 23.4 ms for PMD band measurements. Viewing angles Ψ corresponding to the individual PMD readouts (R_{PMD} + 1 values per scan) are derived from the viewing angles ψ on the 93.75 ms grid of the scanner(R_ψ + 1 values per scan) by linear interpolation as follows (this is similar to the determination of the UTC time grid in A2.3.2):

$\Psi_j = \psi_{j/4} \qquad (j = 0, 4, \ldots, 256)$	*Equation 159*
$\Psi_j = (\Psi_{j-2} + \Psi_{j+2})/2 \qquad (j = 2, 6, \ldots, 254)$	*Equation 160*
$\Psi_j = (\Psi_{j-1} + \Psi_{j+1})/2 \qquad (j = 1, 3, \ldots, 255)$	*Equation 161*

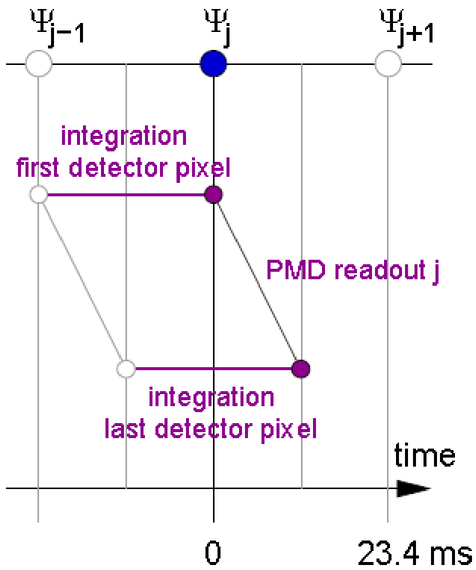

Figure 10: Correspondence between viewing angles and first/last detector pixel.

Due to the finite duration of the integration (23.4 ms) and the readout (11.7 ms), one integration actually covers a range of viewing angles. Assuming that the first scanner readout in a packet coincides with the start of the first PMD readout, the choice of the viewing angles made here is representative of the end of the integration time of the first PMD detector pixel read, or the middle of the integration time of the last detector pixel read, as shown in Figure 10.

Note that $P_{ss,\psi}$, $\cos(2\chi_{ss,\psi})$, $\chi_{ss,\psi}$, $q_{ss,\psi}$, and $u_{ss,\psi}$ are calculated from P_{ss}^{Ψ}, $\cos(2\chi_{ss}^{\Psi})$, $\sin(2\chi_{ss}^{\Psi})$, χ_{ss}^{Ψ}, q_{ss}^{Ψ}, u_{ss}^{Ψ} in a manner analogous to that used for PMD viewing angles as described above.

If *pmd_readout* = *solar* the appropriate solar zenith angle *Zen* and solar azimuth angle *Az* are calculated from the set of basic geolocation parameters calculated in Calculate Geolocation for Fixed Grid (A2.6) and provided in the level 1a product, θ_{Sun} and φ_{Sun}. These basic geolocation parameters are provided on a fixed 187.5 ms integration time grid. See Section 5.2.8. For each readout, the angles from the previous 187.5 ms period should be selected, i.e., angle $n - 1$ corresponds to readout n. This is similar to the selection of angles in Apply Polarisation Correction (A3.10). For PMD readouts in raw transfer mode, the packet contains the last of the 16 readouts in the 375 ms therefore the corresponding scanner angles are 4, 8, ... , 16. See Figure 23.

Convert the solar zenith *Zen* to the solar elevation E using Equation 403 in Appendix C.

5.2.23.4.3.2 Calculate Stokes fractions: Set 1 – Stokes fractions for individual PMD readouts (every 23.4 ms)

In this section, Stokes fractions are calculated for every single PMD readout. These Stokes fractions will not be used for polarisation correction of main channel signals later on, but constitute geophysical output on their own.

Loop information: The following calculations will be performed for all PMD readouts j of a scan, and within a readout for all PMD bands i , that is for $j = 0 \ldots R_{PMD} - 1$, $i = 0 \ldots N_{PMD} - 1$. For Earth-shine PMD band measurements this implies $R_{PMD} \times N_{PMD} = 256 \times 15$ times, not considering the bands missing in the reset data packages.

The calculation starts from dark signal and stray light corrected PMD signals. First the PMD signals S^s_{ij}, S^p_{ij} are compared to given threshold values S^s_{req} , S^p_{req} . If they exceed this threshold;

$$S^s_{ij} \cdot IT^s > S^s_{req} \text{ and } S^p_{ij} \cdot IT^p > S^p_{req} \qquad \text{Equation 162}$$

the Stokes fraction q_{ij} can be derived directly from the PMD s and PMD p signals.

If the signals are below the threshold values, a reliable Stokes fraction cannot be determined. In this case q_{ij} shall be set to “undefined” as defined in Section 5. Assuming $F_{MissStokes}$ has been initialised to zero, then if q_{ij} is missing for any of the readouts j set $F_{MissStokes,\,i} = 1$ and $N_{MissStokes,i} = N_{MissStokes,i} + 1$.

For the missing band data in the reset pixels (16 out of 256 PMD readouts for the band + raw transfer mode, 4 out of 256 PMD readouts for the band+mixed transfer mode) Equation 162 and Equation 167 shall not be applied. Instead, Stokes fractions shall be set to “undefined”, but without raising the $F_{MissStokes}$ flag or incrementing the $N_{MissStokes}$ counter, as this behaviour occurs in every scan.

End loop.

Loop information: The following calculations will be performed for all PMD readouts j of a scan.

First interpolate the Müller matrix elements to the viewing angle Ψ_j of PMD readout j yielding $M^1_{(s/p),\,\Psi_j}$, $\mu^2_{is,\,\Psi_j}$, $\mu^2_{ip,\,\Psi_j}$, $\mu^3_{is,\,\Psi_j}$, $\mu^3_{ip,\,\Psi_j}$ using Linear Interpolation (AX.2). The PMD signals S^s_{ij}, S^p_{ij} are then interpolated to the MME spectral grid λ_{MME} using Spline Interpolation (AX.3). Missing PMD block C readouts are ignored as the data will in this case be extrapolated to the MME spectral grid.

End loop.

Loop information: The following calculations will be performed for all PMD readouts j of a scan and for all spectral grid points i of the MME spectral grid.

Next it is necessary to calculate and apply an update to the relative radiometric response of the PMDs using in-flight PMD band data from those special geometries where Stokes fractions are expected to be zero purely from geometrical considerations alone. For all spectral grid points i in the MME spectral grid initialise $M^{qe}_{i\Psi_j}$, $\sigma^{M,qe}_{i\Psi_j}$ and $N^{e}_{i\Psi_j}$ to 0.

If $\left|\cos(2\chi_{SS,\psi_j})\right| < \cos(2\chi_{SS})_{min}$ then determine the following PMD signal ratio correction:

$$M^{qc}_{i\Psi_j} = M^{1}_{(s/p),\, i\Psi_j} - \frac{S^{s,\,MME}_{ij}}{S^{p,\,MME}_{ij}}$$ *Equation 163*

Next evaluate the index *l* for which $\left|\psi^h - \psi_j\right| < \Delta^{h,\,qc}$ for forward scan readouts *j* only. If no *l* satisfies this condition, raise a warning and do nothing. Otherwise, if $M^{qc}_{i\Psi_j} < \overline{M^{qc}_{i\psi^h_l}} + m_{qc}$ and $M^{qc}_{i\Psi_j} > \overline{M^{qc}_{i\psi^h_l}} - m_{qc}$

$$M^{qc}_{i\psi^h_l} = M^{qc}_{i\Psi_j} + M^{qc}_{i\psi^h_l}$$ *Equation 164*

and

$$N^{c}_{i\psi^h_l} = N^{c}_{i\psi^h_l} + 1$$ *Equation 165*

If , $min\left(\overline{N^{c}_{\psi^h}}\right) \geq N^{qc}$ where $\overline{N^{c}_{\psi^h}}$ is the average of $N^{c}_{i\psi^h_l}$ over all spectral grid points *i* for each high resolution viewing angle *l*, or if an updated correction has not been generated for $\Delta^{t,\,qc}$ days then calculate the mean correction $\overline{M^{qc}_{i\psi^h_l}}$ and the standard deviation $\sigma^{M,\,qc}_{i\psi^h_l}$ from all $N^{c}_{i\psi^h_l}$ stored readouts for which $\overline{N^{c}_{\psi^h_l}} \geq N^{qc}$. Store both the updated correction and the standard deviation in the COR file.

Reset $M^{qc}_{i\psi^h_l}$, $\sigma^{M,\,qc}_{i\psi^h_l}$ and $N^{c}_{i\psi^h_l}$ to zero for those readouts for which $\overline{N^{c}_{\psi^h_l}} \geq N^{qc}$. Next, interpolate $\overline{M^{qc}_{\psi^h}}$ to the viewing angle ψ_j of PMD readout *j* using Linear Interpolation (AX.2) where $\overline{M^{qc}_{\psi^h}}$ is the most recent value from the COR file, yielding $\overline{M^{qc}_{i\Psi_j}}$. Apply this correction to the PMD radiometric response ratio as:

$$M^{1c}_{(s/p),\, i\Psi_j} = M^{1}_{(s/p),\, i\Psi_j} - \overline{M^{qc}_{i\Psi_j}}$$ *Equation 166*

The Stokes fractions are then calculated from the interpolated values $M^{1}_{(s/p),\, i\Psi_j}$, $\mu^2_{is,\,\Psi_j}$, $\mu^2_{ip,\,\Psi_j}$, $\mu^3_{is,\,\Psi_j}$, $\mu^3_{ip,\,\Psi_j}$, the interpolated PMD signals $S^{s,MME}_{ij}$, $S^{p,MME}_{ij}$, and the single-scattering Stokes fraction ratios u_{SS}/q_{SS} only if $\left|q_{SS,\Psi_j}\right| \geq q_{SS,min}$:

$$q^{MMe}_{ij} = \frac{M^{1c}_{(s/p),\, i\Psi_j} - \dfrac{S^{s,MME}_{ij}}{S^{p,MME}_{ij}}}{\left(\mu^2_{ip,\,\Psi_j} + \mu^3_{ip,\,\Psi_j}\dfrac{u_{SS,\,\Psi_j}}{q_{SS,\,\Psi_j}}\right)\cdot\dfrac{S^{s,MME}_{ij}}{S^{p,MME}_{ij}} - \left(\mu^2_{is,\,\Psi_j} + \mu^3_{is,\,\Psi_j}\dfrac{u_{SS,\,\Psi_j}}{q_{SS,\,\Psi_j}}\right)\cdot M^{1c}_{(s/p),\, i\Psi_j}}$$ *Equation 167*

For the "C-shape" region where $\left|q_{SS,\Psi_j}\right| < q_{SS,min}$ the Stokes fraction is calculated as follows:

$$q^{MME}_{ij} = \frac{(1+\mu^3_{ip,\,\Psi_j}\cdot u_{ij}) - (1+\mu^3_{is,\,\Psi_j}\cdot u_{ij})\cdot M^{1c}_{(s/p),\, i\Psi_j}\cdot S^{p,MME}_{ij}/S^{s,MME}_{ij}}{S^{p,MME}_{ij}/S^{s,MME}_{ij}\cdot M^{1c}_{(s/p),\, i\Psi_j}\cdot \mu^2_{is,\,\Psi_j} - \mu^2_{ip,\,\Psi_j}}$$ *Equation 168*

where u is determined as follows:

- If $count(where(\left|q_{SS,\Psi_j}\right| < q_{SS,min})) > 2$ calculate both for the forward and backward scan separately the readout indices which bound the "C-shape", excluding the PMD reset pixels

$$a = min(where(\left|q_{SS,\Psi_j}\right| < q_{SS,min})) - 1 \text{ and}$$ *Equation 169*

$$b = max(where(\left|q_{SS,\Psi_j}\right| < q_{SS,min})) + 1$$ *Equation 170*

- Next Calculate

$$P^a_i = \sqrt{q^2_{ia} + \left(\frac{u_{SS,\,a}}{q_{SS,\,a}}\cdot q_{ia}\right)^2} \text{ and}$$ *Equation 171*

$$P^b_i = \sqrt{q^2_{ib} + \left(\frac{u_{SS,\,b}}{q_{SS,\,b}}\cdot q_{ib}\right)^2}$$ *Equation 172*

- For $j = a,b$ calculate the following:

$$P^x_{ij} = m_{2j}\cdot\frac{P^a_i}{P_{ss,\,a}}\cdot P_{ss,j} + m_{1j}\cdot\frac{P^b_i}{P_{ss,\,b}}\cdot P_{ss,j}$$ *Equation 173*

where $m_2 = 0$ if a does not exist and $m_1 = 0$ if b does not exist and otherwise:

$$m_{1j} = \frac{j-a}{b-a} \text{ and } m_{2j} = \frac{b-j}{b-a}$$ *Equation 174*

- Finally for $j = a,b$ calculate the following:

$$u_{ij} = P^{\chi}_{ij} \cdot \sin 2\chi_{ss,j}$$ *Equation 175*

If *pmd_readout* = *solar* interpolate the Muller matrix elements to the viewing angle Ψ_s of the Sun measurement yielding $M^{1}_{(s/p),\Psi_s}$, μ^{2}_{is,Ψ_s}, μ^{2}_{ip,Ψ_s} using Linear Interpolation (AX.2).

The Sun Stokes fractions are then as:

$$q^{Sun,MME}_{ij} = \frac{M^{1c}_{(s/p),i\Psi_s} - \dfrac{S^{s,MME}_{ij}}{S^{p,MME}_{ij}}}{\mu^{2}_{ip,\Psi_s} \cdot \dfrac{S^{s,MME}_{ij}}{S^{p,MME}_{ij}} - \mu^{2}_{is,\Psi_s} \cdot M^{1c}_{(s/p),i\Psi_s}}$$ *Equation 176*

The error in the Stokes fractions stored in MDR-1*-Earthshine: POL_M Q_POL_ERR shall be set to “undefined”.

End of loop.

The Stokes fractions calculated as described above are then interpolated from q^{MME} and $q^{Sun,\,MME}$ back to the original wavelength grid of PMD p to yield q and q^{Sun} using Spline Interpolation (AX.3).

5.2.23.4.3.3 Calculate Stokes fractions: Set 2 – Stokes fractions for main channel correction (every 187.5 ms)

For main channel polarisation correction (A3.10), Stokes fractions representative of the main channel integration time are required. They are calculated here from the ratios of averaged PMD signals.

Note: It can be shown that simply averaging the individual Stokes fractions from the previous step is not equivalent and does in fact not give the correct result.

For a 187.5 ms main channel integration time, eight PMD readouts of 23.4 ms have to be averaged. To take into account the finite readout time of FPA and PMD channels, four of these averages have to be calculated per main channel integration time, each shifted by one PMD readout with respect to the next. (This will become evident in algorithm A3.10.1. See Figure 15. This gives a total of $4 \times 32 = 128$ Stokes fractions per PMD band and scan. The selection of PMD readouts to be averaged for a given FPA readout follows the synchronisation between FPA and PMD channels (see also Figure 13 in Appendix C) such that $\bar{q}_{\text{[illegible]}}$ can be used in A3.10 for correction of main channel readout

n. The very first FPA integration in a scan coincides with the last PMD readouts of the previous scan, so they have to be accessible here.

Loop information: The following calculations will be performed for all 187.5 ms subpixels n of a scan, for all PMD averages m i.e., for $n = 0 \ldots R_{FPA} - 1$, $m = 0 \ldots 3$, and for all points i in the MME spectral grid.

For given n, m, the average viewing angle $\overline{\Psi}$ and average PMD signals $\overline{S^{s,MME}}$, $\overline{S^{p,MME}}$ are calculated considering the eight PMD readouts from $j_1 = 8(n-1) + m$ to $j_2 = j_1 + 7$, where a negative readout index j corresponds to PMD readout $R_{PMD}+j$ from the previous scan:

$$\overline{\Psi} = \frac{1}{8}\sum_{j=j_1}^{j_2} \Psi_j, \quad \overline{S^{s,MME}} = \frac{1}{8}\sum_{j=j_1}^{j_2} S_{ij}^{s,MME}, \quad \overline{S^{p,MME}} = \frac{1}{8}\sum_{j=j_1}^{j_2} S_{ij}^{p,MME}$$

Equation 177

If no previous scan is available, the Stokes fractions for the affected readout are set to “undefined”. The $F_{\text{MissStokes}}$ flag and $N_{\text{MissStokes}}$ counter shall not be changed as they are reserved for set 1 of the Stokes fractions.

Similarly to the previous step (Set 1), the Müller matrix elements are then linearly interpolated to the viewing angle $\overline{\Psi}$.

Then interpolate $\overline{M^{qc}_{\Psi^h}}$ to the viewing angle $\overline{\Psi}$ where $\overline{M^{qc}_{\Psi^h}}$ is the most recent value from the COR file yielding $\overline{M^{qc}_{i\Psi}}$ and apply this correction to the PMD radiometric response ratio as follows:

$$M^{1c}_{(s/p),\, i\overline{\Psi}} = M^{1}_{(s/p),\, i\overline{\Psi}} - \overline{M^{qc}_{i\overline{\Psi}}}$$

Equation 178

The Stokes fraction is calculated from the interpolated values $M^{1c}_{(s/p),\, i\overline{\Psi}}$, $\mu^2_{is,\overline{\Psi}}$, $\mu^2_{ip,\overline{\Psi}}$, $\mu^3_{is,\overline{\Psi}}$, $\mu^3_{ip,\overline{\Psi}}$, the averaged PMD signals $\overline{S^{s,MME}}$, $\overline{S^{p,MME}}$, and the single scattering Stokes fraction ratios u_{SS}/q_{SS} as follows:

$$\overline{q^{MME}_{imn}} = \frac{M^{1c}_{(s/p),\, i\overline{\Psi}} - \dfrac{\overline{S^{s,MME}}}{\overline{S^{p,MME}}}}{\left(\mu^2_{ip,\overline{\Psi}} + \mu^3_{ip,\overline{\Psi}}\dfrac{u_{SS,n-1}}{q_{SS,n-1}}\right) \cdot \dfrac{\overline{S^{s,MME}}}{\overline{S^{p,MME}}} - \left(\mu^2_{is,\overline{\Psi}} + \mu^3_{is,\overline{\Psi}}\dfrac{u_{SS,n-1}}{q_{SS,n-1}}\right) \cdot M^{1c}_{(s/p),\, i\overline{\Psi}}}$$

Equation 179

For the “C-shape” region where $|q_{SS,n-1}| < q_{SS,min}$ the Stokes fraction is calculated as follows:

$$\overline{q_{imn}^{MME}} = \frac{(1+\mu^3_{ip,\overline{\Psi}} \cdot u_{mn}) - (1+\mu^3_{is,\overline{\Psi}} \cdot u_{mn}) \cdot M^{1c}_{(s/p),i\overline{\Psi}} \cdot \dfrac{\overline{S_{ij}^{p,MME}}}{\overline{S_{ij}^{s,MME}}}}{\dfrac{\overline{S_{ij}^{p,MME}}}{\overline{S_{ij}^{s,MME}}} \cdot M^{1c}_{(s/p),i\overline{\Psi}} \cdot \mu^2_{is,\overline{\Psi}} - \mu^2_{ip,\overline{\Psi}}}$$

Equation 180

where u is determined as follows:

- If $count(where(|q_{SS,n-1}| < q_{SS,min})) \neq 0$ calculate both for the forward and backward scan separately the readout indices which bound the “C-shape”, excluding the PMD reset pixels.

$$a = min(where(|q_{SS,n-1}| < q_{SS,min})) - 1 \text{ and}$$

Equation 181

$$b = max(where(|q_{SS,n-1}| < q_{SS,min})) + 1$$

Equation 182

For $n = a,b$ calculate the following:

$$u_{mn} = \frac{1}{8} \cdot \sum_{j=j_1}^{j=j_2} u_{ij} \text{ with}$$

Equation 183

$j_1 = 8(n-1) + m$ to $j_2 = j_1 + 7$, where a negative readout index j corresponds to PMD readout $R_{PMD} + j$ from the previous scan. If no previous scan is available the u-Stokes fractions shall be set to “undefined”.

Again, the Stokes fractions $\overline{q^{MME}}$ calculated as described above are interpolated back to the original wavelength grid of PMD p to yield $\overline{q}$ using Spline Interpolation (AX.3).

If due to missing data in the reset pixels less than four PMD band readouts are available for the sum, Equation 177 and Equation 179 shall not be applied. Stokes fractions $\overline{q}_{imn}$ shall be set to “undefined”. This condition implies the following:

- in the band + raw transfer mode, Stokes fractions $\overline{q}_{imn}$ cannot be calculated for two out of the 32 (= R_{FPA}) 187.5 ms subpixels,
- in the band+mixed transfer mode, Stokes fractions $\overline{q}_{imn}$ can be calculated for all subpixels, as there are never more than four PMD readouts missing.

End of loop.

5.2.23.4.4 Determine PCDs From Stokes Fractions (A2.21.5)

Missing Stokes fractions have already been flagged above.

Stokes fractions from set 2 are flagged “bad” if they are not between the unpolarised (q = 0) and the single-scattering ($q = q_{SS}$) value (allowing some margin δq). The check is only performed if the scattering angle can be assumed to be constant with wavelength. This is the case if the single-scattering degree of polarisation is not too low or the wavelength is high enough. The detailed procedure is as follows:

Initialise all elements of $F_{\mathrm{BadStokes}}$ to 0.

Loop information: The following calculations will be performed for all 187.5 ms subpixels n of a scan, for all PMD averages m, and for all PMD bands i, for $n = 0 \ldots R_{FPA} - 1$, $m = 0 \ldots 3$, $i = 0 \ldots N_{PMD} - 1$.

In the following, $\mathrm{sign}(x) \equiv \begin{cases} +1 & (x \geq 0) \\ -1 & (x < 0) \end{cases}$

If $(P_{SS,\,n-1} > P_{SS,\,\mathrm{min,\,BadStokes}}$ or $\lambda_i > \lambda_{\mathrm{min,\,BadStokes}})$ and
$(\mathrm{sign}(q_{SS,\,n-1})\bar{q}_{imn} < -\delta q$ or $\mathrm{sign}(q_{SS,\,n-1})(\bar{q}_{imn} - q_{SS,\,n-1}) > \delta q)$, set $F_{\mathbf{BadStokes},in} = 1$.

Note: Associating single-scattering degree of polarisation and Stokes fraction $n - 1$ with the Stokes fraction for main channel readout n ensures correct synchronisation between the two quantities.

End of loop.

For all those PMD bands i ($i = 0 \ldots N_{PMD} - 1$) where $F_{\mathrm{BadStokes},in} = 1$ for at least one subpixel n, increment the global counter $N_{\mathrm{BadStokes},i}$ by 1.

Finally, the scene variability within 187.5 ms subpixels is calculated as the normalised standard deviation of the PMD signals (sum over both PMD detectors) for PMD band i_{Scene}:

Loop information: The following calculations will be performed for all 187.5 ms subpixels n of a scan, for $n = 0 \ldots R_{FPA} - 1$.

Calculate the average PMD signal (sum over both PMD detectors) as follows:

$$\bar{S}_{\mathbf{Scene}} = \frac{1}{8} \sum_{j=8n}^{8n+7} (S^p_{i_{\mathrm{Scene}},j} + S^s_{i_{\mathrm{Scene}},j})$$

Equation 184

and the scene variability as follows:

$$\sigma_{\mathbf{Scene},\,n} = \frac{1}{\bar{S}_{\mathbf{Scene}}} \sqrt{\frac{1}{7} \sum_{j=8n}^{8n+7} (S^p_{i_{\mathrm{Scene}},j} + S^s_{i_{\mathrm{Scene}},j} - \bar{S}_{\mathbf{Scene}})^2}$$

Equation 185

For the special case of $\bar{S}_{\mathbf{Scene}} = 0$, set $\sigma_{\mathbf{Scene},n} = 0$, in order to avoid division by zero.

For PMD reset pixels (see Appendix B), set $\sigma_{\mathbf{Scene},n} = 0$ to "undefined".

End of loop.

5.2.24 COLLECT GLOBAL PCDs PER PRODUCT (A2.22)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One product assumed to be 'dump to dump'.

5.2.24.1 Objective

To collect all global PCDs at the completion of processing of one complete product, assumed in this context to be 'dump to dump'. The PQE functionality will also make use of these global PCDs.

5.2.24.2 Description

All global PCDs, indicated in the variable tables by the type 'g', are collected at the completion of processing of one complete product, assumed in this context to be 'dump to dump'. Global PCDs are typically flags indicating non-nominal behaviour and cumulative counts of the number of occurrences of non-nominal behaviour. Information describing observation mode statistics is also included. Global PCDs will be written in the level 1a and subsequently the level 1b product.

5.2.24.3 Variables

5.2.24.3.1 Global PCDs per product

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/ Remarks*
N_{scan}	Number of scans in the product	w	-	g/o	A2.0.7/A2.23.3	**SPHR** N_SCANS
N_{val_dp}	Number of valid scans with missing data packets	w	-	g/o	A2.0.7/A2.23.3	**SPHR** N_VALID_WITH_MISS_DP
N_{miss_dp}	Number of missing data packets invalid scans	w	-	g/o	A2.0.7/A2.23.3	**SPHR** N_MISS_DP
N_{miss_scan}	Number of missing scans	w	-	g/o	A2.0.7/A2.23.3	**SPHR** N_MISSING_SCANS
N_{nn_dt}	Number of scans with non-nominal detector temperature	w[B]	-	g/o	A2.2/A2.23.3	**SPHR** N_NN_DETECTOR_TEMP
N_{nn_pdp}	Number of scans with non-nominal pre-disperser prism temperature	w	-	g/o	A2.2/A2.23.3	**SPHR** N_NN_PDP_TEMP
N_{nn_rad}	Number of scans with non-nominal radiator temperature	w	-	g/o	A2.2/A2.23.3	**SPHR** N_NN_RAD_TEMP
N_{nn_WLSU}	Number of scans with non-nominal WLS lamp voltage	w	-	g/o	A2.2/A2.23.3	**SPHR** N_NN_WLS_U
N_{nn_WLSI}	Number of scans with non-nominal WLS lamp current	w	-	g/o	A2.2/A2.23.3	**SPHR** N_NN_WLS_I
N_{nn_SLSU}	Number of scans with non-nominal SLS lamp voltage	w	-	g/o	A2.2/A2.23.3	**SPHR** N_NN_SLS_U
N_{nn_SLSI}	Number of scans with non-nominal SLS lamp current	w	-	g/o	A2.2/A2.23.3	**SPHR** N_NN_WLS_I
N_{inv_UTC}	Number of scans with invalid UTC	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_INV_UTC

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
N_{Nad_scan}	Number of scans in *Nadir_scan* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_NADIR_SCAN
N_{Nth_scan}	Number of scans in *Nth_pole_scan* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_NTH_POLE_SCAN
N_{Sth_scan}	Number of scans in *Sth_pole_scan* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_STH_POLE_SCAN
N_{Oth_scan}	Number of scans in *Other_scan* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_OTHER_SCAN
N_{Nad_static}	Number of scans in *Nadir_static* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_NADIR_STATIC
N_{Oth_static}	Number of scans in *Other_static* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_OTHER_STATIC
N_{Dark}	Number of scans in *Dark* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_DARK
N_{LED}	Number of scans in *LED* observation mode	w	-	g/o	A2.3.1/lv1a	**SPHR** N_LED
N_{WLS}	Number of scans in *WLS* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_WLS
N_{SLS}	Number of scans in *SLS* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_SLS
N_{SLS_diff}	Number of scans in *SLS* over diffuser observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_SLS_DIFF
N_{Sun}	Number of scans in *Sun* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_SUN
N_{Moon}	Number of scans in *Moon* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_MOON
N_{Idle}	Number of scans in *Idle* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_IDLE
N_{Test}	Number of scans in *Test* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_TEST

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/ Remarks
N_{Dump}	Number of scans in *Dump* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_DUMP
$N_{Invalid}$	Number of scans assigned an *Invalid* observation mode	w	-	g/o	A2.3.1/A2.23.3	**SPHR** N_INVALID
N_{sat}	Number of scans with saturated pixels	w[B]	-	g/o	A2.4.1/A2.23.3	**SPHR** N_SATURATED
N_{hot}	Number of scans with hot pixels	w[B]	-	g/o	A2.4.2/A2.23.3	**SPHR** N_HOT
N_{min}	Number of scans where the mean uncalibrated signal is below a specified threshold per band	w[B]	-	g/o	A2.4/A2.23.3	**SPHR** N_MIN_INTENSITY
N_{SAA}	Number of scans in the SAA	w	-	g/o	A2.7.1/A2.23.3	**SPHR** N_SAA
$N_{sunglint}$	Number of scans with sunglint danger	w	-	g/o	A2.7.2/A2.23.3	**SPHR** N_SUNGLINT
$N_{rainbow}$	Number of scans with rainbow danger	w	-	g/o	A2.7.3/A2.23.3	**SPHR** N_RAINBOW
$N_{mode,geo}$	Number of scans with possible mismatch between observation mode and geolocation	w	-	g/o	A2.7.3/A2.23.3	**SPHR** N_MODE_GEOLOCATION
$N_{\mathrm{MissStokes}}$	Number of scans with missing Stokes fractions	$w[N_{\mathrm{PMD}}]$	-	g/o	A2.22	**SPHR** N_MISS_STOKES
$N_{\mathrm{BadStokes}}$	Number of scans with bad Stokes fractions	$w[N_{\mathrm{PMD}}]$	-	g/o	A2.22	**SPHR** N_BAD_STOKES

5.2.24.4 Algorithm

All of the global PCDs listed in Section 5.2.24.3 are collated and passed to Write Level 0 and 1a Product (A2.23) to be formatted in the level 1a product as specified in [AD 4] and [AD 5].

5.2.25 WRITE LEVEL 0 AND 1A PRODUCT (A2.23)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One product assumed to be ‘dump to dump’.

5.2.25.1 Objective

To collate and write all information to be written to the level 1a product and level 0 product header as specified in [AD 4] and [AD 5].

5.2.25.2 Description

All information to be included in the level 1a product, and additional header information to be included in the level 0, is collated and formatted as specified in [AD 4] and [AD 5]. Specific references to fields contained within [AD 4] and [AD 5] are included in the variable tables in this Chapter.

5.2.25.3 Variables

As defined in [AD 4] and [AD 5] and referenced previously in variable tables.

5.2.25.4 Algorithm

5.2.25.4.1 Generate Level 0 and 1a Data Records (A2.23.1)

The level 0 data records consist of Instrument Science Data Packets. The level 1a data records consist of the contents of the MDR-1a data records as specified in [AD 4] and [AD 5].

5.2.25.4.2 Generate In-Flight Calibration Data Records (A2.23.2)

The in-flight data records consist of the contents of the VIADR-1a-* data records specified in[AD 4] and [AD 5]. Note that for internal calculations using the in-flight data records double precision should be used rather than the scaled integers used in the output product format.

5.2.25.4.3 Generate Header and Global Product Information (A2.23.3)

The header and global product information consists of the MPHR, SPHR, GEADR-*, GIADR-*data records specified in [AD 4] and [AD 5].

5.3 LEVEL 1A TO 1B PROCESSING (A3)

5.3.1 Processing Overview

Figure 11, Figure 12, Figure 13, and Figure 14 show the second level of decomposition for the functional box A3. They provide an overview of required interfaces and the processing flow. The following description concentrates on the input and output data. The processor receives the following input data:

Initialisation data
This data set contains all parameter settings for the PGF, such as threshold values, switches between algorithm options, and instrument parameters not contained in the instrument key data.

Static auxiliary data
The static auxiliary data comprises the static databases that are required for use in the level 1a to 1b processor. They are required in particular for the effective cloud cover and cloud top pressure determination.

Key data
The Key data comprise the complete set of pre-flight calibration data which is provided by the instrument provider. Only stray light characterisation parameters are required for the level 1a to 1b processor.

GOME-2 level 1a data stream
Level 1a data stream comprises in addition to the housekeeping and raw binary data as contained in the level 0 the instrument science packets, geolocation information on a fixed grid, all in-flight calibration data and Müller Matrix Elements required by the level 1a to 1b processor.

The PGF generates the following output:

GOME-2 level 1b data stream
Depending on the time coverage of the level 1a data stream on input the generated level 1b data stream covers the corresponding time period. The level 1a to 1b processor generates the Level 1b data stream for formatting as specified in [AD 4] and [AD 5]. These data will be stored in the EUMETSAT Data Centre and are available for reprocessing purposes.

A summary of the applicable processing steps for all observation modes and configurable options for the processor is given in Appendix A.

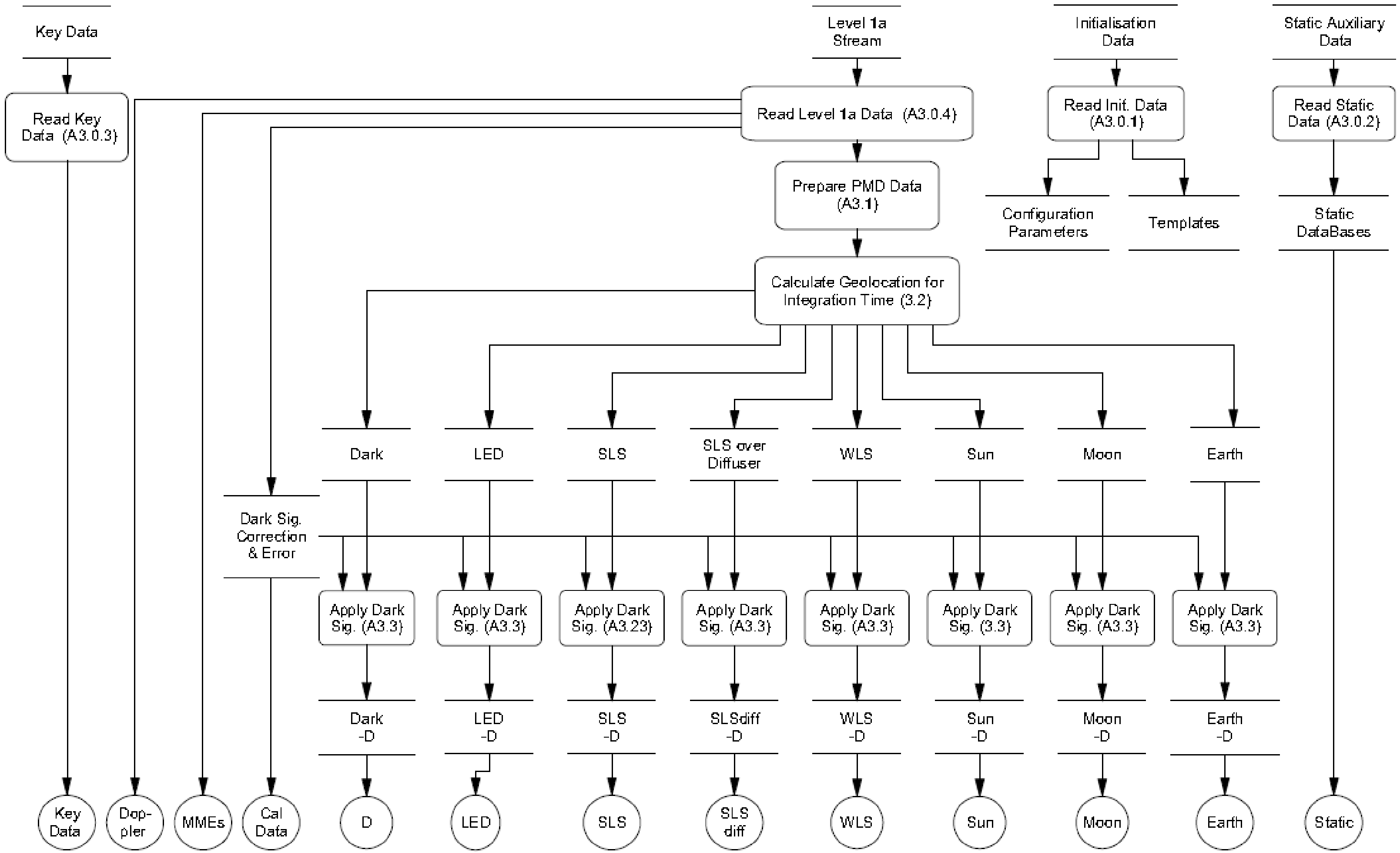

Figure 11: A3 Functional Decomposition: Level 1a to 1b Processor (1).

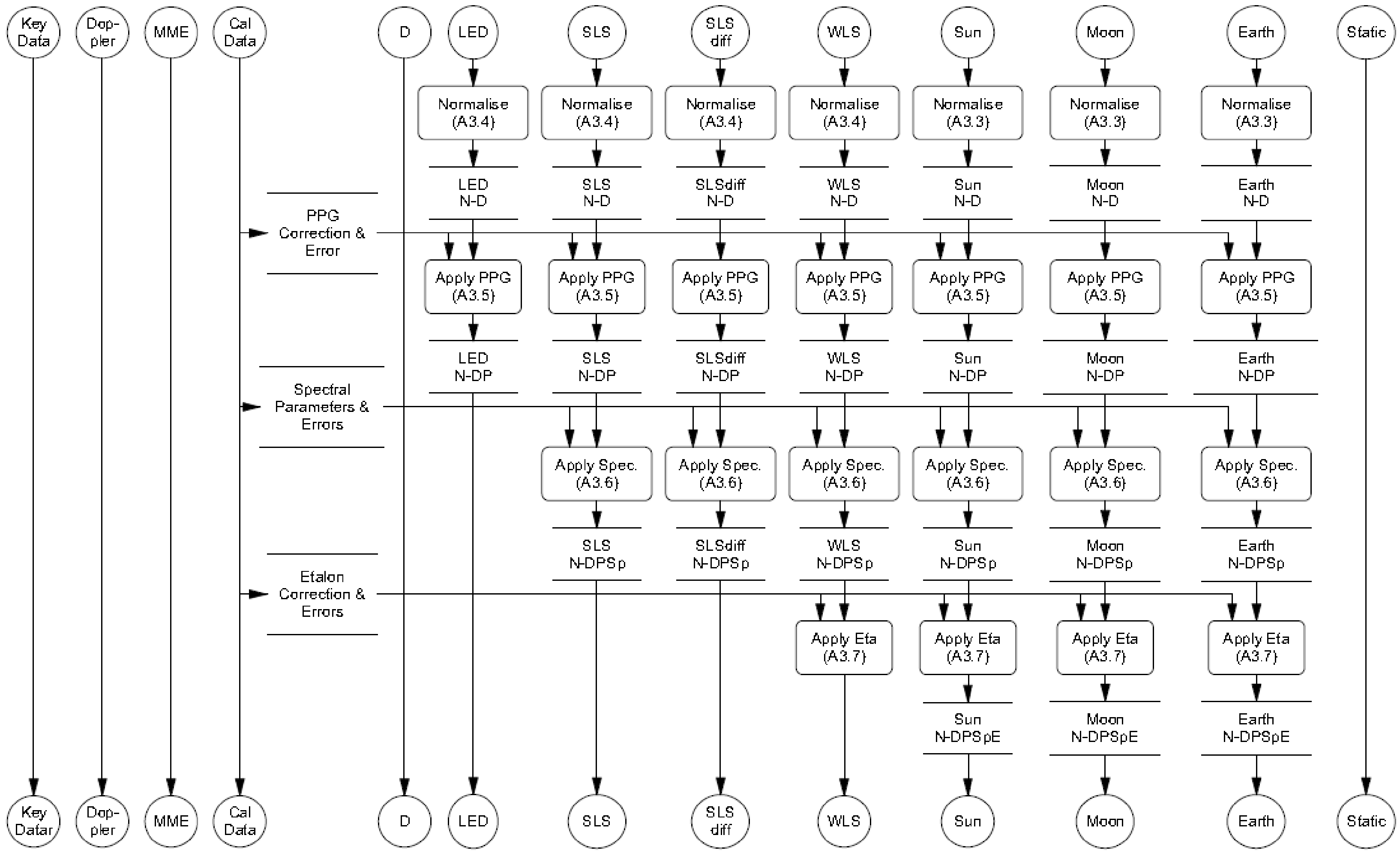

Figure 12: A3 Functional Decomposition: Level 1a to 1b Processor

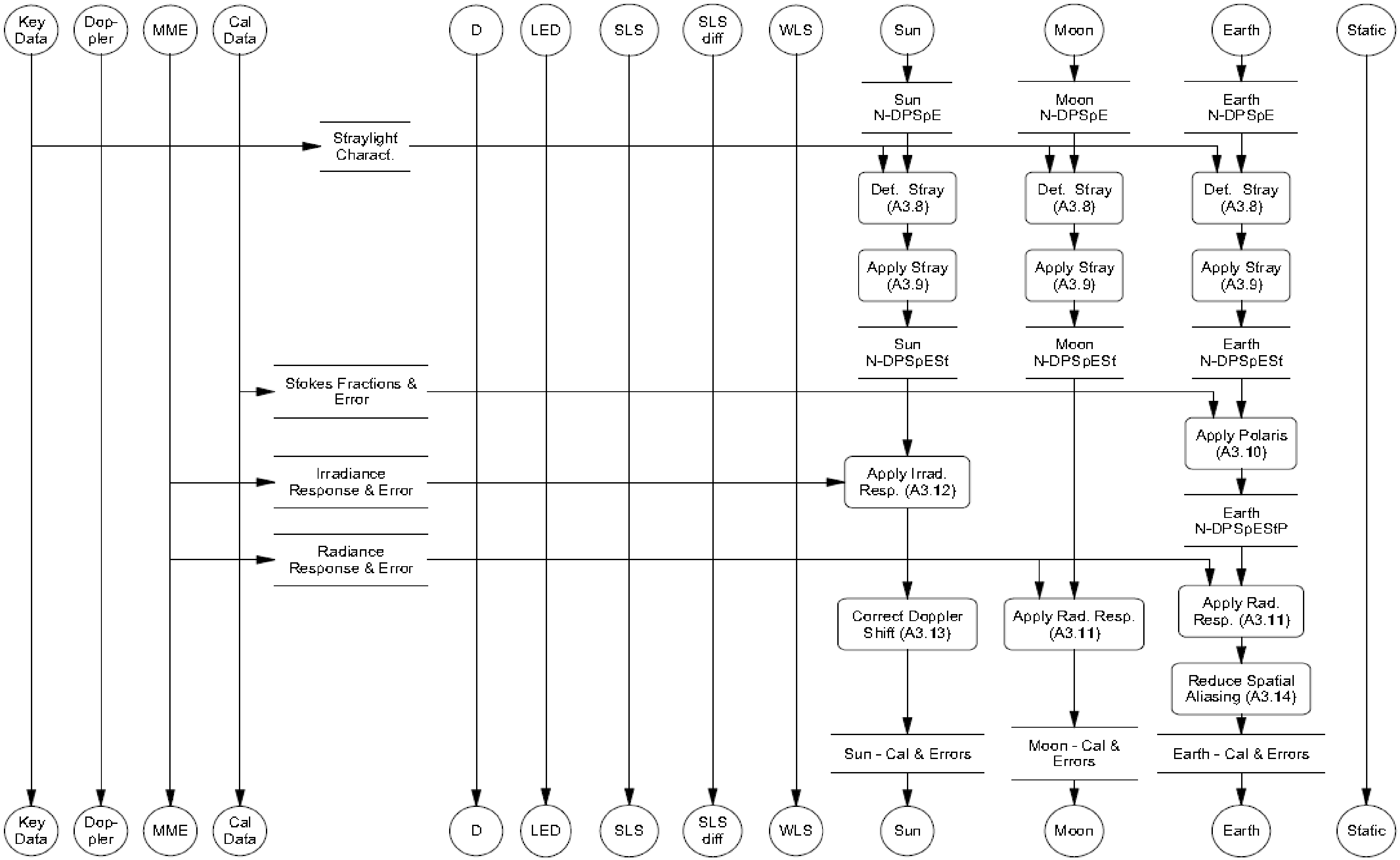

Figure 13: A3 Functional Decomposition: Level 1a to 1b (3)

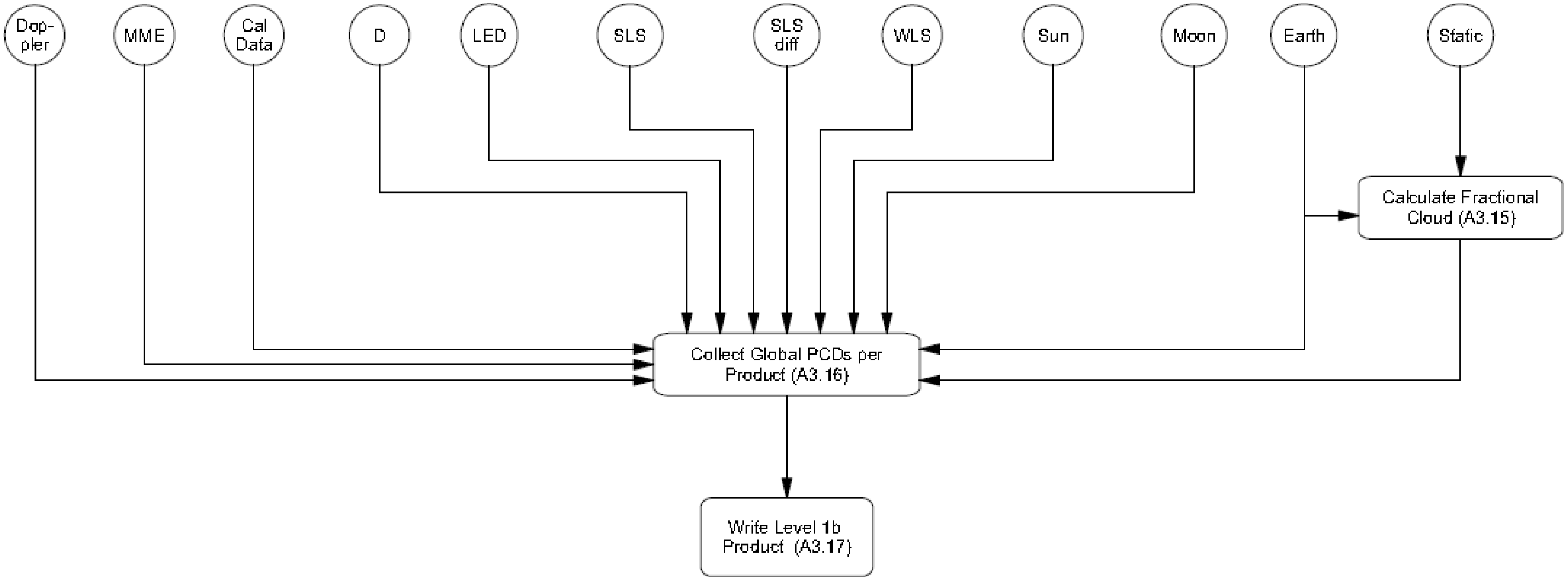

Figure 14: A3 Functional Decomposition: Level 1a to 1b Processor (4)

5.3.2 Read Input Data

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

Initialisation Data
Static Auxiliary Data
Key Data
In-flight Calibration Data
Level 1a Data Product or Stream

5.3.2.1 Objective

To read all input data required by the GOME-2 level 1a to 1b processor.

5.3.2.2 Description

This module reads all initialisation data, static auxiliary data, key data and in-flight calibration data required by the GOME-2 level 1a to 1b processor. In addition, the level 1a data product is read and separated into individual scans for further processing.

5.3.2.3 Variables

5.3.2.3.1 Read Initialisation Data (A3.0.1)

The initialisation data set used in the generation of a level 1b product is referenced in record **GEADR-Initialisation** as specified in [AD 5].

5.3.2.3.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*References/Remarks*
δ_{dt}	Dark signal detector temperature tolerance	d	K	i/o	ini/A3.3	*0.2*
SAA_{pix}	Band 1a detector pixel number for SAA correction estimate	i	-	i/o	ini/A3.3	*5*
SAA_{sort}	Number of band 1a detector pixels to be sorted for SAA correction estimate	i	-	i/o	ini/A3.3	*50*
SAA_{1a}	Flag indicating whether to apply the additional dark signal correction to band 1a measurements in the SAA	bool	-	i/o	ini/A3.3	*1 = correct* *0 = do not correct*
pe	Number of photo-electrons per BU for each channel	i[B]	BU^{-1}	i/o	ini/ ini/A3.3, A3.11	*960*
δ_{PPG}	PPG error estimate for each channel	d[]	-	i/o	ini/A3.5	*0.001*
δ_{pdp}	Pre-disperser prism temperature tolerance	d	K	i/o	ini/A3.6	*0.2*
M	Order of wavelength calibration polynomial per channel	i[B]	-	i/o	ini/A3.6 and various	*3, 3, 4, 4, 6, 6*
δ_{Eta}	Etalon error estimate for each channel	d[B]	-	i/o	ini/A3.7	*0.01*
δ_{Stray}	Stray light error estimate for each channel	d[B]	-	i/o	ini/A3.9	*0.01*
δ_{Pol}	Polarisation correction error estimate for each channel	$d[B_{FPA}]$	-	i	ini/A3.10	*0.01*
N_{PMD}	Total number of PMD bands	w	-	i/o	ini/A3.10 and various	*15*
δ_{rd}	Readout time per detector pixel	d	s	i/o	ini/A3.10 and A3.14	45.776367×10^{-6}
$SunNorm$	Switch indicating whether to calculate the absolutely calibrated radiance or a sun-normalised radiance	enum	-	i/o	ini/A3.11	*AbsRad* (see [AD5])
c	Speed of light	d	m/s	i/o	ini/A3.13	$2.99792458 \cdot 10^{8}$
Δt_{sm}	Offset for first scanner position relative to UTC date/time stamp in Science Data Packet	d	s	i/o	ini/A3.14	*–0.375*
λ^{alias}	Wavelength to be used for association of a PMD band with each main channel	$d[B_{FPA}]$	nm	i/o	ini/A3.14	*280.0, 360.0, 500.0,700.0*

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	References/Remarks
N_{coadd}	Number of sets of co-added PMD readouts needed to cover the main channel readout time.	i	-	i/o	ini/A3.14	*4 This will change if the ratio of main channel to PMD integration time changes*
λ_{alias}	Four wavelengths used for Akima extrapolation in the “Reduce Spatial Aliasing” algorithm	d[4]	nm	i/o	ini/A3.14	*[100,150,900,950]*
Δ_{depol}	Depolarisation parameter for Rayleigh scattering	d	-	i/o	ini/A3.15	*0.0657,* valid at 290 nm [GD 6]
t_{cloud}	Threshold for effective fractional cloud cover	d	-	i/o	ini/A3.15	*0.1*
t_{UV}	UV albedo threshold for snow/ice	d	-	i/o	ini/A3.15	*0.2*
A_S^{sea}	Assumed surface albedo over sea	d	-	i/o	ini/A3.15	*0.02*
A_c	Lambertian cloud albedo	d	-	i/o	ini/A3.15	*0.8*
c_{fg}	First guess effective cloud fraction	d		i/o	ini/A3.15	*0.5*
z_{cfg}	First guess cloud top height	d	km	i/o	ini/A3.15	*5*
A_{fg}	First guess albedo of lower reflecting boundary for retrieval in the presence of snow/ice.	d	-	i/o	ini/A3.15	A_c
z_{fg}	First guess height of lower reflecting boundary for retrieval in the presence of snow/ice.	d	km	i/o	ini/A3.15	*zs*
$\delta\chi^2$	Cut-off for variation in χ^2	d	-	i/o	ini/A3.15	*0.1*
ε_{Rsim}	Relative error in simulated reflectivity	d	-	i/o	ini/A3.15	
θ_0^{max}	Maximum allowed Solar Zenith Angle	d	degree	i/o	ini/A3.15	*85*
R_{max}	Maximum allowed reflectivity	d	-	i/o	ini/A3.15	*1.2*
λ_{cont}	Wavelength outside the oxygen-A band representing continuum absorption only	d	nm	i/o	ini/A3.15	*758*
maxiter	Maximum number of iterations for cloud parameter retrieval	i	-	i/o	ini/A3.15	*10*

5.3.2.3.3 Read Static Auxiliary Data (A3.0.2)

The static auxiliary data sets used in the generation of a level 1b product are referenced in record **GEADR-Static** as specified in [AD5].

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*References/Remarks*
NE_{lat}	Number of latitudes in elevation dataset	i	-	i/o	stat/A3.15	
NE_{lon}	Number of longitudes in elevation dataset	i	-	i/o	stat/A3.15	
E_{lat}	Latitude grid for *Elev*	$d[NE_{lat}]$	degree	i/o	stat/A3.15	
E_{lon}	Longitude grid for *Elev*	$d[NE_{lon}]$	degree	i/o	stat/A3.15	
Elev	Elevation	$d[NE_{lat}, NE_{lon}]$	m	i/o	stat/A3.15	

The static auxiliary data sets used in the generation of a level 1b product are referenced in record **GEADR-Static** as specified in [AD5].

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
N_{lev}	Number of atmospheric levels in simulations	i	-	i/o	stat/A3.15	
z^{stat}	Grid for height of atmospheric layers in simulations	$d[N_{lev}]$	km	i/o	stat/A3.15	
p^{stat}	Grid for pressure of atmospheric layers in simulations	$d[N_{lev}]$	hPa	i/o	stat/A3.15	
N_{coef}	Number of polynomial coefficients for expansion of transmittance	i	-	i/o	stat/A3.15	*nominal value 4*
N^{ref}	Number of wavelengths for which α is parameterised and for cloud parameter fitting.	i	-	i/o	stat/A3.15	*nominal value 15*
N_{θ}	Number of viewing angles for which α is parameterised	i	-	i/o	stat/A3.15	
N_{θ_0}	Number of solar zenith angles for which α is parameterised	i	-	i/o	stat/A3.15	
λ^{ref}	Wavelength grid for which α is parameterised	$d[N_{\lambda}]$	nm	i/o	stat/A3.15	
θ^{stat}	Viewing angle grid for which α is parameterised	$d[N_{\theta}]$	degree	i/o	stat/A3.15	
θ_0^{stat}	Solar zenith angle grid for which α is parameterised	$d[N\theta_0]$	degree	i/o	stat/A3.15	
α	Polynomial coefficients for calculation of transmittance	$d[N_{coef}, N_{\lambda}, N_{\theta}, N\theta_0]$	-	i/o	stat/A3.15	
β	Polynomial coefficients for calculation of Rayleigh single-scattering reflectance	$d[N_{coef}, N_{\lambda}, N_{\theta}, N\theta_0]$	-	i/o	stat/A3.15	

The static auxiliary data sets used in the generation of a level 1b product are referenced in record GEADR-Static as specified in [AD 5].

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
NR_{lat}	Number of latitudes in minimum reflectivity dataset	i	-	i/o	stat/A3.15	
NR_{lon}	Number of longitudes in minimum reflectivity dataset	i	-	i/o	stat/A3.15	
NR_{λ}	Number of wavelengths in mini-mum reflectivity dataset	i	-	i/o	stat/A3.15	*nominal value 2*
λ^{R}	Wavelength grid for R_{min}	d[NR_{λ}]	nm	i/o	stat/A3.15	*nominal values* λ = 758 *nm and* λ = 772 *nm*
R_{lat}	Latitude grid for R_{min}	d [NR_{lat}]	deg	i/o	stat/A3.15	
R_{lon}	Longitude grid for R_{min}	d[NR_{lon}]	deg	i/o	stat/A3.15	
R_{min}	Minimum reflectivity dataset	d[NR_{λ}, NR_{lat}, R_{lon}]	-	i/o	stat/A3.15	*from GOME/ERS-2 data approximately 1 x 1 degree resolution*

5.3.2.3.4 READ KEY DATA (A3.0.3)

The Key Data set used in the generation of a level 1b product is referenced in record **GEADR-KeyData** as specified in [AD 5].

5.3.2.3.4.1 Input from key dataset: Key data for stray light calculation

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
F	Uniform stray light fraction per channel (intra-channel only)	d[B]	-	i/o	key/AG.16	
N^{G}	Number of stray light ghosts for each channel	i[B]	-	i/o	key/AG.16	
I	Polynomial coefficients describing the intensity of stray light ghosts	d[3,N^{G},B]	-	i/o	key/AG.16	
p	Polynomial coefficients describing the location of stray light ghosts	d[3,N^{G},B]	-	i/o	key/AG.16	

5.3.2.4 Algorithm

5.3.2.4.1 Read Initialisation Data (A3.0.1)

The Initialisation Data listed in Section 5.3.2.3 are read from the Initialisation Data storage location and made available for use in Level 1a to 1b Processing (A3).

5.3.2.4.2 Read Static Auxiliary Data (A3.0.2)

The Static Auxiliary Data listed in Section 5.3.2.3 are read from the Static Auxiliary Data storage location and made available for use in Level 1a to 1b Processing (A3).

5.3.2.4.3 Read Key Data (A3.0.3)

The Key Data listed in Section5.3.2.3 are read from the Key Data storage location and made available for use in Preprocess Müller Matrix Elements (A2.1).

5.3.2.4.4 Read Level 1a Input Data (A3.0.4)

The level 1a data stream or product, formatted as specified in [AD4] and [AD5], is read and made available for use in Level 1a to 1b Processing (A3).

5.3.3 PREPARE PMD DATA (A3.1)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark	√	FPA	
Sun	√	Housekeeping	
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other			

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.4 CALCULATE GEOLOCATION FOR ACTUAL INTEGRATION TIMES (A3.2)

Instrument Modes		Instrument Data	
Earth	√	PMD	
Dark		FPA	
Sun		Housekeeping	√
WLS			
SLS			
SLS over Diffuser			
LED			

Uses Generic Sub-Function:
Calculate Geolocation for Fixed Grid (AG.2)
Calculate Centre Coordinates (AG.20).
Uses Auxiliary Sub-Functions:
None
Data Granule
One Scan, with access to previous scans.

5.3.4.1 Objective

Calculate the geolocations for the ground pixels corresponding to the actual main channel integration times from the geolocations for the fixed 187.5 ms grid and also for PMD integration times based on calculations from high resolution scanner angle positions.

5.3.4.2 Description

For measurements in the earth observation modes, this module derives geolocation parameters for the various main channel integration times in a scan from the geolocation parameters for the fixed 187.5 ms grid which have been calculated in module Calculate Geolocation for Fixed Grid (A2.6). The synchronisation between main channel readouts and level 1a 187.5 ms ground pixels (see Figure 23) is taken into account. Geolocations refer to the first detector pixel read in a main channel. All parameters are calculated from geolocation parameters given in the level 1a product. PGE services related to geolocation (orbit propagation) are not required. For PMD data with 3M's integration time the geolocation is calculated from high resolution scanner angle positions. In the special case of earth observation mode PMD data, geolocation information will be calculated using the formula in *Calculate Geolocation for Fixed Grid* found in AG.2.

Scanner viewing angles will be calculated for the middle of the actual integration time. As in A2.6, latitude and longitude values will be calculated for corner points ABCD and centre point F. Solar and satellite zenith and azimuth angles will be calculated for points E and G at the sides of the ground pixel and centre point F. The same convention for labelling the ground pixel points is used, looking in flight direction, points AEB are always on the left, and points CGD are always on the right, independent of the scan direction (see Figure 21). Geolocation parameters for actual integration times will be denoted by an *a* in their name.

Example: *lon* is the longitude for the fixed (187.5 ms) integration time from A2.6 and *alon* is the longitude for the actual integration time calculated below. θ_{Sun} is the solar zenith angle for the fixed integration time, θ_{aSun} is the solar zenith angle for the actual integration time.

Assumption on integration times: Integration times have been chosen in such a way that either the scan mirror does not reverse its direction during integration or the integration covers one or more complete scans:

- Integration times below 6 s (the scan duration) are selected such that 1.5 s (the duration of the back scan) is an integer multiple of the integration time. These integration times are compatible with this assumption: 93.75 ms, 187.5 ms, 375 ms, 0.75 s, 1.5 s.
- Integration times of 6 s and more are integer multiples of 6 s.

For integration times not fulfilling these assumptions, actual geolocations will *not* be computed.

GOME-2 main channel data cannot be down linked more often than every 187.5 ms. For the *shortest main channel integration time*, 93.75 ms, the instrument provides therefore *two commandable options*:

- No co-adding: Every second 93.75 ms spectrum is recorded in the data packet; the other one is discarded.
- Co-adding: Two 93.75 ms spectra are co-added by the on-board software. The result is divided by two and recorded in the science data packet.

It is indicated per band in the Science Data Packet which of the two options has been selected. For the purpose of this module, there is no difference between the 93.75 ms integration time with co-adding and the 187.5 ms integration time: they cover the same ground scene. The integration time 93.75 ms with co-adding will therefore be treated as integration time 187.5 ms.

5.3.4.3 Variables

5.3.4.3.1 *Indices*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
i	Index of scan mirror readout within scan corresponding to readout with a given integration time	*i*	-	*t*	-	Starting from 0.
k	Integration time index	*i*	-	*t*	-	
m	Index of completed readout with a given integration time within scan	*i*	-	*t*	-	Starting from 0.
n_{Start}	First 187.5 ms ground pixel from level 1a covered by readout with a given integration time	*i*	-	*t*	-	
n_{Mid}	First 187.5 ms ground pixel from level 1a in the second half of readout with a given integration time above 187.5 ms	*i*	-	*t*	-	
n_{End}	Last 187.5 ms ground pixel from level 1a covered by readout with a given integration time	*i*	-	*t*	-	
N_{Start}	First scan covered by readout with a given integration time	*i*	-	*t*	-	Current scan is 0, previous scans have negative indices
N_{End}	Last scan covered by readout with a given integration time	*i*	-	*t*	-	

5.3.4.3.2 *Local Variables*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
integration_start	Start of integration relative to scan duration	d	s	t	-	
integration_end	End of integration relative to scan duration	d	s	t	-	
T_f	Integration time corresponding to individual level 1a ground pixels which are combined to form level 1b ground pixels (187.5 ms or 6 s)	d	s	t	-	
$t_{\psi PMD}$	UTC time associated with the scanner angle grid for PMD geolocation with an additional element at the end of a scan.	d[$R_{\phi,\mathrm{PMD}}$+1]	days	t	-	$R_{\psi,PMD} = 0...511$

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	Remarks
ψ_{PMD}	High resolution scanner angle grid for PMD geolocation,	d[$R_{\phi,PMD}$ +1]	-	*t*	-	$R_{\psi,PMD} = 0...511$

5.3.4.3.3 Input from level 1a data stream or other functions

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
mode	Observation mode	enum	-	i	A3.0.4	**MDR-1*** OBSERVATION_MODE
pmd_transfer	PMD transfer mode	enum	-	i	A3.0.4	**MDR-1*** PMD_TRANSFER
IT_{FPA}	Integration times for main channel bands (some elements may be equal)	d[B]	s	i	A3.0.4	**MDR-1a-** INTEGRATION_TIMES
UTC	UTC time associated with every second scanner position	d[32]	days	i	A3.0.4	**MDR-1a-Earthshine** GEO_BASICUTC_TIME
ψ	Scanner viewing angle with additional element at end of scan	d[R_{ϕ}+1]	degree	i	A3.0.4	**MDR-1a-**SCANNER_ANGLE
slon	Geocentric longitude for complete scan, ground, points ABCDF (earth-fixed CS)	d[5]	degree	i	A3.0.4	**MDR-1a-Earthshine** GEO_EARTH SCAN_CORNER & SCAN_CENTRE
slat	Geodetic latitude for complete scan, ground, points ABCDF (earth-fixed CS)	d[5]	degree	i	A3.0.4	**MDR-1a-Earthshine** GEO_EARTH SCAN_CORNER & SCAN_CENTRE
lon	Geocentric longitude, ground, points ABCDF (earth-fixed CS)	d[R_{FPA},5] *or* d[R_{PMD},5]	degrees	i	A3.0.4 *or* AG.2	**MDR-1a-Earthshine** GEO_EARTH CORNER & CENTRE
lat	Geodetic latitude, ground, points ABCDF (earth-fixed CS)	d[R_{FPA},5] *or* d[R_{PMD},5]	degrees	i	A3.0.4 *or* AG.2	**MDR-1a-Earthshine** GEO_EARTH CORNER & CENTRE
φ_{Sun}	Solar azimuth, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degrees	i	A3.0.4 *or* AG.2	**MDR-1a-Earthshine** GEO_EARTH SOLAR_AZIMUTH

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
θ_{Sun}	Solar zenith, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	i	A3.0.4 *or* AG.2	**MDR-1a-Earthshine** GEO_EARTH SOLAR_ ZENITH
φ_{Sat}	Satellite azimuth, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	i	A3.0.4 *or* AG.2	**MDR-1a-Earthshine** GEO_EARTH SAT_AZIMUTH Earth mode only
θ_{Sat}	Satellite zenith, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	i	A3.0.4 *or* AG.2	**MDR-1a-Earthshine** GEO_EARTH SAT_ZENITH Earth mode only

5.3.4.3.4 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
N_{IT}	Number of unique integration times in scan	b	-	o	A3.17.1	**MDR-1b-Earthshine** N_UNIQUE_INT
IT	Unique integration times in scan	d[N_{IT}]	s	o	A3.17.1	**MDR-1b-Earthshine** UNIQUE_INT

scan_direction	Scanning direction	enum [R_{FPA}] *or* enum d[R_{PMD}]	-	o	A3.17.1	**MDR-1b-Earthshine** GEO_EARTH_ACTUAL_ #SCAN_DIRECTION
						0 = other
						1 = forward
						2 = backward

readout_start_time	UTC time associated with the readout of the detector pixel which is read out first in each band.	enum [R_{FPA}] *or* enum d[R_{PMD}]	days	o	A3.17.1	**MDR-1b-Earthshine** GEO_EARTH_ACTUAL_ #READOUT_START_TIME
Ψ_a	Scanner viewing angle corresponding to middle of actual integration time	d[R_{FPA}] *or* d[R_{PMD}]	degree	o	A3.17.1	**MDR-1b-Earthshine** GEO_EARTH_ACTUAL_# SCANNER_ANGLE_ACTUAL

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*Remarks*
alon *alat*	Geocentric longitude corresponding to actual integration time, ground, points ABCDF (earth-fixed CS)	d[R_{FPA},5] *or* d[R_{PMD},5]	degree	o	A3.17.1	**MDR-1b-Earthshine** GEO_EARTH_ACTUALCORNER_ ACTUAL and CENTRE_ACTUAL For integration times greater than 187.5 ms, only the first *M* entries of the first dimension will be filled, where *M* is the number of readouts for that integration time.
φ_{aSun}	Solar azimuth corresponding to actual integration time, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	o	A3.15/A3.17.1	**MDR-1b-Earthshine** GEO_EARTH SOLAR_ AZIMUTH Earth mode only *res*[66]
θ_{aSun}	Solar zenith corresponding to actual integration time, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	o	A3.15/A3.17.1	**MDR-1b-Earthshine** GEO_EARTH SOLAR ZENITH Earth mode only
φ_{aSat}	Satellite azimuth corresponding to actual integration time, *h*0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	o	A3.15/A3.17.1	**MDR-1b-Earthshine** GEO_EARTH SAT_AZIMUTH *res*[8]
θ_{aSat}	Satellite zenith corresponding to actual integration time, *h*0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	o	A3.15/A3.17.1	**MDR-1b-Earthshine** GEO_EARTH SAT_ZENITH

5.3.4.4 Algorithm

5.3.4.4.1 Calculate Geolocation for Actual Integration Times For FPAs (A3.2.1)

Some of the integration times for the six main channel bands (1a, 1b, 2a, 2b, 3, 4) may have the same value. Find the *NIT* unique integration times IT_k ($k = 0 \ldots N_{IT} - 1$). Treat bands having an integration time of 93.75 ms with co-adding as if they would have an integration time of 187.5 ms. See Case 2 below. Exclude integration times not compatible with the assumptions above from the unique integration times.

Note: When information from a previous scan is not accessible (because the current scan is the first scan, or because a previous scan is missing), the corresponding output parameters (the ones which cannot be calculated because of missing data) are set to “undefined” and the flag for degraded MDR quality due to a processing degradation (DEGRADED_PROC_MDR) is raised.

Loop information: Do the following for the N_{IT} unique integration times IT_k ($k = 0 \ldots N_{IT} - 1$), and within a unique integration time, for all readouts *m* belonging to this integration time within the scan.

Note: The level 1a ground pixel referred to below is the 187.5 ms ground pixel from A2.6. Within a scan, *m* and *n* start from zero. Negative indices *n* correspond to ground pixel $R_{FPA} + n$ from the previous scan. Negative scanner viewing angle indices *i* correspond to viewing angle $R_{\psi} + i$ from the previous scan. For a given integration time IT_k, *m* is counting the *completed* readouts only, $m = 0, 1, 2, \ldots$ (and *not*, 0, 2, 4, … for $IT_k = 375$ ms). Unused elements of actual geolocation parameters shall be set to “undefined”. E.g., for $IT_k = 1.5$ s only the first four elements of the first dimension are filled, and the remaining $R_{FPA} - 4$ elements are set to “undefined”.

Case 1: $IT_k = 93.75$ ms without co-adding

Note: As in this case only every second readout is inserted in the science data packet, there are 32 (*not 64)* completed readouts in a 6 s scan, $m = 0, 1, 2, \ldots, 31$.

Start and end ground pixel are the same:

$$n_{\text{start}} = n_{\text{end}} = m - 1$$

Equation 186

Assign the scanner viewing angle corresponding to the middle of the readout:

$$\psi_{a,\,mk} = (\psi_{2m-1} + \psi_{2m})/2$$

Equation 187

a. Static modes

If the observation mode *mode* is static (nadir static or other static), the difference between a 187.5 ms ground pixel and a 93.75 ms ground pixel is so small that it can safely be neglected. Define *alon*, *alat* (points ABCDF), φ_{aSun}, θ_{aSun}, φ_{aSat}, θ_{aSat} (points EFG) by assigning them the corresponding points from the start/end ground pixel. E.g., set $\varphi_{aSun,mEk} = \varphi_{Sun,m-1,E}$.

b. Scanning modes

Otherwise (the observation mode is one of the scanning modes), the actual geolocation of a 93.75 ms ground pixel will be the “second half” of a 187.5 ms ground pixel. We have to distinguish between forward scan and back scan.

If $0 \leq n_{\text{start}} < 24$ (forward scan), the “second half” is the “right half”:

- Point A: Call module Calculate Centre Coordinates (AG.20), providing longitude/latitude values for points A and C of the start/end ground pixel, $lon_{m-1,A}$, $lat_{m-1,A}$, $lon_{m-1,C}$, $lat_{m-1,C}$, on input. The module will provide coordinates $alon_{mAk}$, $alat_{mAk}$ on output.
- Point B: Call module Calculate Centre Coordinates (AG.20), providing longitude/latitude values for points B and D of the start/end ground pixel, $lon_{m-1,B}$, $lat_{m-1,B}$, $lon_{m-1,D}$, $lat_{m-1,D}$, on input. The module will provide coordinates $alon_{mBk}$, $alat_{mBk}$ on output.
- Points CD: Use points CD of the start/end ground pixel. E.g., set $alon_{mCk} = lon_{m-1,C}$.
- Point E: For the solar and satellite zenith and azimuth angles, use point F (!) of the start/end ground pixel. E.g., set $\varphi_{aSun,mEk} = \varphi_{Sun,m-1,F}$.
- Point G: For the solar and satellite zenith and azimuth angles, use point G of the start/end ground pixel.
- Point F: Call module Calculate Centre Coordinates (AG.20), providing newly calculated actual longitude/latitude values for points B and C, $alon_{mBk}$, $alat_{mBk}$, $alon_{mCk}$, $alat_{mCk}$, on input. The module will provide coordinates $alon_{mFk}$, $alat_{mFk}$ on output. For the solar and satellite zenith and azimuth angles, use the arithmetic mean of the newly calculated actual angles at points E and G–set $\varphi_{aSun,mFk} = (\varphi_{aSun,mEk} + \varphi_{aSun,mGk})/2$.

If $n_{\text{start}} < 0$ or $n_{\text{start}} \geq 24$ (back scan), the “second half” is the “left half”:

- Points AB: Use points AB of the start/end ground pixel. E.g., set $alon_{mAk} = lon_{m-1,A}$.
- Point C: Call module Calculate Centre Coordinates (AG.20), providing longitude/latitude values for points A and C of the start/end ground pixel, $lon_{m-1,A}$, $lat_{m-1,A}$, $lon_{m-1,C}$, $lat_{m-1,C}$, on input. The module will provide coordinates $alon_{mCk}$, $alat_{mCk}$ on output.
- Point D: Call module Calculate Centre Coordinates (AG.20), providing longitude/latitude values for points B and D of the start/end ground pixel, $lon_{m-1,B}$, $lat_{m-1,B}$, $lon_{m-1,D}$, $lat_{m-1,D}$, on input. The module will provide coordinates $alon_{mDk}$, $alat_{mDk}$ on output.
- Point E: For the solar and satellite zenith and azimuth angles, use point E of the start/end ground pixel.
- Point G: For the solar and satellite zenith and azimuth angles, use point F (!) of the start/end ground pixel. Set $\varphi_{aSun,mGk} = \varphi_{Sun,m-1,F}$.
- Point F: as above for the forward scan.

Case 2: 187.5 ms $\le IT_k$ < 6s (including IT_k = 93.75 ms with co-adding)

In this case, the geolocations *lon*, *lat* of the 187.5 ms level 1a ground pixels are used for the calculation of geolocations *alon*, *alat* for the actual integration times.

Determine the index of the scan mirror readout corresponding to the middle of readout of integration time IT_k as follows, where $T_f = 187.5 \times 10^{-3}$ s.

$$i = \frac{IT_k}{T_f}(2m-1)$$ *Equation 188*

Assign the scanner viewing angle corresponding to the middle of readout of integration time IT_k:

$$\Psi_{a,mk} = \Psi_i$$ *Equation 189*

Determine the indices of the first and last level 1a ground pixel covered by the readout of integration time IT_k as follows, where again $T_f = 187.5 \times 10^{-3}$ s.

$$\text{Start ground pixel: } n_{\text{start}} = \frac{IT_k}{T_f}(m-1)$$ *Equation 190*

$$\text{End ground pixel: } n_{\text{end}} = \frac{IT_k}{T_f}m - 1$$ *Equation 191*

If IT_k > 187.5 ms, calculate also the first ground pixel of the second half of IT_k:

$$n_{\text{mid}} = n_{\text{start}} + (n_{\text{end}} - n_{\text{start}} + 1)/2$$ *Equation 192*

Notes: See Figure 23.

1. This choice refers to the *first* detector pixel read in a channel.
2. For $m = 0$ this gives $n_{\text{end}} = -1$: For all integration times, the first readout in a scan ends with the last ground pixel in the previous scan.
3. For IT_k = 187.5 ms this associates level 1a ground pixel $m - 1$ with readout m. This implies that even for IT_k = 187.5 ms the geolocation for the fixed grid (level 1a) and the geolocation for the actual integration time (level 1b) will differ. This is because the geolocation for the fixed grid is related to scanner positions while the geolocation for the actual integration time is given for the scene observed during the integration.
4. The total number of level 1a ground pixels covered by a readout of integration time IT_k is this:

$$n_{\text{end}} - n_{\text{start}} + 1 = \frac{IT_k}{T_f}.$$

According to the assumptions on integration times, this number is 1, 2, 4, or 8.

To select the four corner coordinates $alon_{mAk}$, $alat_{mAk}$,…, $alon_{mDk}$, $alat_{mDk}$, and the start/end solar and satellite zenith and azimuth angles $\varphi_{aSun,mEk}$, $\varphi_{aSun,mGk}$, $\theta_{aSun,mEk}$, $\theta_{aSun,mGk}$, $\varphi_{aSat,mEk}$, $\varphi_{aSat,mGk}$, $\theta_{aSat,mEk}$, $\theta_{aSat,mGk}$, for the *m*th ground pixel with integration time IT_k we have to distinguish between forward scan and back scan:

If $0 \le n_{\text{start}} < 24$ and $0 \le n_{\text{end}} < 24$ (forward scan), the two corner points AB from the start ground pixel and the two corner points CD from the end ground pixel form the corner points ABCD of the ground pixel *m* for integration time IT_k. Point E from the start ground pixel and point G from the end ground pixel are selected as points E and G of the ground pixel *m* for integration time IT_k.

If $n_{\text{end}} < 0$ or $n_{\text{start}} \ge 24$ (back scan), the two corner points AB from the end ground pixel and the two corner points CD from the start ground pixel form the corner points ABCD of the ground pixel *m* for integration time IT_k. Point E from the end ground pixel and point G from the start ground pixel are selected as points E and G of the ground pixel m for integration time IT_k.

Determine the (approximate) scan centre point F by a call to module Calculate Centre Coordinates (AG.20), providing coordinates of points B and C, $alon_{mBk}$, $alat_{mBk}$, $alon_{mCk}$, $alat_{mCk}$ on input. The module will provide centre coordinates $alon_{mFk}$, $alat_{mFk}$ on output.

Finally, the centre solar and satellite zenith and azimuth angles $\varphi_{aSun,mFk}$, $\theta_{aSun,mFk}$, $\varphi_{aSat,mFk}$, $\theta_{aSat,mFk}$, have to be calculated:

- If $IT_k = 187.5$ ms, use the corresponding angles for point F from the start ground pixel n_{start}.
- Otherwise ($IT_k > 187.5$ ms), if $0 \le n_{\text{start}} < 24$ and $0 \le n_{\text{end}} < 24$ (forward scan), use the arithmetic mean of the angles from point G of ground pixel $n_{\text{mid}} - 1$ and point E of ground pixel n_{mid}. (This accounts for the finite extension of the instantaneous field-of-view in across-track direction.) For example, set $\varphi_{aSun,mFk} = (\varphi_{Sun,nmid-1,G} + \varphi_{Sun,nmidE})/2$. If $n_{\text{end}} < 0$ or $n_{\text{start}} \ge 24$ (back scan), use the arithmetic mean of the angles from point E of ground pixel $n_{\text{mid}} - 1$ and point G of ground pixel n_{mid}.

Case 3: $IT_k \ge 6$s

In this case we have, at most, one readout in the scan. As integration times are integer multiples of 6s, we use the geolocations *slon*, *slat* for the scan as a whole here.

If there is no readout in the scan, set all actual geolocations corresponding to IT_k to “undefined”.

If there is a readout in the scan, determine the corner points as follows.

Determine the indices of the first and last scan covered by the readout of integration time IT_k as follows, where $T_f = 6$ s, scan 0 is the current scan, scan –1 the previous scan, etc.

$$\text{Start scan: } N_{\text{start}} = -\frac{IT_k}{T_f}$$ *Equation 193*

$$\text{End scan: } N_{\text{end}} = -1$$ *Equation 194*

The scan corner points A from the end scan, B from the start scan, C from the end scan and D from the start scan form the corner points ABCD of the ground pixel m for integration time IT_k (coordinates $alon_{mAk}$, $alat_{mAk}$,…, $alon_{mDk}$, $alat_{mDk}$).

As in cases 1 and 2, determine the (approximate) scan centre point F by a call to module Calculate Centre Coordinates (AG.20), providing coordinates of points B and C, $alon_{mBk}$, $alat_{mBk}$, $alon_{mCk}$, $alat_{mCk}$, on input. The module will provide centre coordinates $alon_{mFk}$, $alat_{mFk}$ on output.

The middle of the forward part of the end scan is assigned to the actual viewing angle:

$$\Psi_{a,mk} = \Psi_{24}\big|_{N_{\text{end}}}$$ *Equation 195*

For these large ground pixels it is not possible to define truly representative solar and satellite angles. Therefore, the following approximations will be used for φ_{aSun}, θ_{aSun}, φ_{aSat}, θ_{aSat}:

- Point E: Use the arithmetic mean of the angles for point E of readout 0 of the start scan and point E of readout 31 of the end scan. For example, calculate $\varphi_{aSun,mEk}$ as $\varphi_{aSun,mEk} = (\varphi_{Sun,0,E|N\text{start}} + \varphi_{Sun,31,E|N\text{end}})/2$.
- Point F: Use the arithmetic mean of the angles for point E of readout 12 of the start scan, and point G of readout 28 of the end scan.
- Point G: Use the arithmetic mean of the angles for point G of readout 24 of the start scan and point G of readout 24 of the end scan.

End of loop.

5.3.4.4.2 CALCULATE GEOLOCATION FOR ACTUAL INTEGRATION TIMES FOR PMDS (A3.2.2)

Geolocation information for actual integration times is for PMDs only calculated for block D and E data (see Section B on page 400). For blocks D and E, PMD data is read out at a fixed integration time of 23.4375 ms resulting in 256 completed readouts in one scan, N_{PMD} = 0...255.

A fine scanner angle grid with $2N_{PMD} + 1$ elements ψ_{PMD} is calculated from the nominal scanner angle Ψ using Linear Interpolation (AX.2). Next, calculate UTC times appropriate to these scanner angles as follows. First interpolate the UTC times provided in the level 1a product for every second scanner position to every scanner position as described in Equation 36, Equation 37, and Equation 38. Then, using the UTC times calculated for every scanner position, calculate $t_{\psi,PMD}$ using Linear Interpolation (AX.2).

If *pmd_transfer = band* or *pmd_transfer = mixed* then the PMD geolocation parameters synchronised with every second point of the fine PMD scanner angle grid, are calculated from ψ_{PMD} and using Calculate Geolocation for Fixed Grid (AG.2).

Note: For PMD readout m, the scanner angle associated with the middle of the actual integration time is calculated as $\psi_{a,m} = \psi_i$ where $i = 2m – 1$.

Additionally $n = m – 1$ such that the first readout in a scan ends with the last ground pixel in the previous scan. Therefore $alon_{mA}$, $alat_{mA}$,…, $alon_{mD}$, $alat_{mD}$, and the start/end solar and satellite zenith and azimuth angles $\varphi_{aSun,mE}$, $\varphi_{aSun,mG}$, $\theta_{aSun,mE}$, $\theta_{aSun,mG}$, $\varphi_{aSat,mE}$, $\varphi_{aSat,mG}$, $\theta_{aSat,mE}$, $\theta_{aSat,mG}$, for the mth ground pixel are given by lon_{nA}, lat_{nA},…, lon_{nD}, lat_{nD}, and the start/end solar and satellite zenith and azimuth angles $\varphi_{Sun,nE}$, $\varphi_{Sun,nG}$, $\theta_{Sun,nE}$, $\theta_{Sun,nG}$, $\varphi_{Sat,nE}$, $\varphi_{Sat,nG}$, $\theta_{Sat,nE}$, $\theta_{Sat,nG}$. Similarly, the centre solar and satellite zenith and azimuth angles $\varphi_{aSun,mF}$, $\theta_{aSun,mF}$, $\varphi_{aSat,mF}$, $\theta_{aSat,mF}$, correspond to $\varphi_{Sun,nF}$, $\theta_{Sun,nF}$, $\varphi_{Sat,nF}$, $\theta_{Sat,nF}$.

In the case that *pmd_transfer = raw* (with an integration time of 375 ms), the same calculation is performed as for the *pmd_transfer = band* or *pmd_transfer = mixed* except that from the results only every 16th readout starting with an offset of 15 is written to the level 1b product.

5.3.4.4.3 Determine Readout Start Time and Scan Direction (A3.2.3)

Loop information: Do the following for the N_{IT} unique integration times IT_k ($k = 0 \ldots N_{IT} - 1$), and within a unique integration time, for all readouts *m* belonging to this integration time within the scan. Note that the effective integration time should be used in case of co-adding.

Calculate *intergration_end* 0.1875 × (*m* – 1). In the case of PMD data, calculate *integration_end* = $(0.1875 \times (int(m_{pmd}/8) - 1)) + (m_{pmd} - (int(m_{pmd}/8) \times 8)) \times IT_{pmd}$.

The *integration_start* is the end of integration – IT_k.

The scan direction is then calculated as follows:

If 0 ≤ integration_start ≤ 4.5 then *scan_direction = forward*

If (integration_start ≤ 0) and (integration_end ≤ 0) and ($IT_k \leq 1.5$) then *scan_direction = backwards*.

If (integration_start ≥ 4.5) and (integration_end ≥ 4.5) and ($IT_k \leq 1.5$) then *scan_direction = backwards*.

Otherwise for *mode = Nadir_static* or *mode = Other_static* then *scan_direction = other*.

Finally, calculate *readout_start_time* by adding *integration_start* to the UTC time of the first scanner position (equivalent to the first data packet in the scan).

End loop.

5.3.5 APPLY DARK SIGNAL CORRECTION (A3.3)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark	√	FPA	√
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other			

Uses Generic Sub-Function:

Apply Dark Signal Correction (AG.11).

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.6 NORMALISE SIGNALS TO ONE SECOND INTEGRATION TIME (A3.4)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark	√	FPA	√
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other			

Uses Generic Sub-Function:

Normalise Signals to One Second Integration Time (AG.12).

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.7 APPLY PPG CORRECTION (A3.5)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon			
Other			

Uses Generic Sub-Function:

Apply PPG Correction (AG.13).

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.8 APPLY SPECTRAL CALIBRATION PARAMETERS (A3.6)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS	√		
SLS	√		

SLS over Diffuser	√		
LED			
Moon	√		
Other			

Uses Generic Sub-Function:

Apply Spectral Calibration (AG.14).

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.9 APPLY ETALON CORRECTION (A3.7)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED			
Moon	√		
Other			

Uses Generic Sub-Function:

Apply Etalon Correction (AG.15)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.10 DETERMINE STRAYLIGHT CORRECTION (A3.8)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon	√		
Other			

Uses Generic Sub-Function:

Determine Stray light Correction (AG.16)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.11 APPLY STRAYLIGHT CORRECTION (A3.9)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon	√		
Other			

Uses Generic Sub-Function:

Apply Stray light Correction (AG.17)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.12 APPLY POLARISATION CORRECTION (A3.10)

Instrument Modes		Instrument Data	
Earth	√	PMD	
Dark		FPA	√
Sun		Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Apply Stray light Correction (AG.17)

Uses Auxiliary Sub-Functions:

Linear Interpolation (AX.2)

Spline Interpolation (AX.3)

Akima Interpolation (AX.4)

Data Granule

One Scan, with access to the previous scan.

5.3.12.1 Objectives

Correct preprocessed earth observation mode main channel signals for the polarisation sensitivity of the instrument.

5.3.12.2 Description

This module corrects signals measured in the main channels in earth observation mode for the polarisation sensitivity of the instrument. This corresponds to converting the signals to signals which would have been observed with an instrument which is not sensitive to the polarisation state of the incoming radiance, or, equivalently, to signals which would have been observed with unpolarised light on input. Applying polarisation correction is a necessary prerequisite for an absolute radiometric calibration of the earth radiances, i.e., for applying the radiance response function (A3.11). Polarisation correction is applied on main channel signals only. PMD signals will be treated differently in module Apply Radiance Response (A3.11).

The module uses the Stokes fractions $\overline{q}$ derived from collocated PMD measurements in module A2.21 characterising the polarisation state of the incoming radiance, single-scattering Stokes fractions u_{SS}, and the Müller matrix elements μ^2 and μ^3 for the main channels, characterising the polarisation sensitivity of the instrument. Main channel signals on input must have been at least dark signal corrected and normalised to one-second integration time.

The algorithm consists of three steps:

1. Establish time correlation between main channels and PMD channels: The relative timing of main channel and PMD readouts is determined from the detector readout time and sequence, and the dispersion relation.

2. Interpolate Stokes fractions to main channel wavelength grid: Four sets of up to 16 Stokes fractions per shortest main channel integration time are provided by Determine Stokes Fractions (A2.21): a theoretical Rayleigh single-scattering value for the UV and one Stokes fraction derived from each of the 15 PMD bands. Each of these values has been assigned a wavelength before. The four sets of Stokes fractions are then interpolated to the much finer wavelength grid of the main channels. For wavelengths below the single-scattering wave-length, main channel Stokes fractions are set to the single-scattering value. For wavelengths above the wavelength of the last valid Stokes fraction, main channel Stokes fractions are set to the last valid Stokes fraction. The four sets of Stokes fractions are interpolated to one set taking into account the relative timing of main channel and PMD readouts.
3. Calculate and apply polarisation correction factors: Stokes fractions on the main channel wavelength grid and main channel Müller matrix elements μ2 and μ3 for the current viewing angle are combined into a polarisation correction factor. The input main channel signals are divided by this polarisation correction factor to yield polarisation corrected signals.

5.3.12.3 Variables

5.3.12.3.1 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
δ_{pol}	Polarisation correction error estimate for each channel	d[B_{FPA}]	-	i	A3.0.1	

5.3.12.3.2 Indices

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*Remarks*
i	PMD band index	i	-	t	-	0…N_{PMD} – 1
k	PMD detector pixel index (blocks CDE)	i	-	t	-	768…1023
m	Index of Stokes fraction set for main channel correction	i	-	t	-	0...3
n	Index number of current 187.5 ms ground pixel within scan	i	-	t	-	0…R_{FPA}–1. Read-out 0 is the first readout in first data packet of the scan.

5.3.12.3.3 Local variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*Remarks*
m^r	Parameter describing relative timing of main channel detector pixel with respect to PMD pixel at the same wavelength (see text for details)	d[D,B_{FPA}]	-	t	-	$0 < m^r < 3$
$m^{r,int}$	integer part of m^r	i[D,B_{FPA}]	-	t	-	0…2
$m^{r,frac}$	fractional part of m^r	d[D,B_{FPA}]	-	t	-	$\leq m^{r,\mathrm{frac}} < 1$
t_{FPA}	time of the readout of FPA detector pixel (after readout of first FPA pixel)	d	s	t	-	
t_{PMD}	time of the readout of PMD detector pixel (after readout of first FPA pixel) for first of the four sets of Stokes fractions	d	s	t	-	
$\hat{q}$	Stokes fractions interpolated to main channel detector pixels, four sets	d[D,B_{FPA},4]	-	t	-	

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*Remarks*
c	Polarisation correction factor for main channel detector pixels	d[D,B_{FPA}]	-	t	-	
N_v	Number of valid Stokes fractions	i	-	t	-	$\leq N_{PMD} + 1$
q_v	Valid Stokes fractions	d[N_v]	-	t	-	
λ_v	Wavelength corresponding to valid Stokes fractions	d[N_v]	nm	t	-	
Ψ	Scanner viewing angle	d	degrees	t	-	

5.3.12.3.4 *Input from initialisation dataset*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
δ_{rd}	Readout time per detector pixel	d	s	i	A3.0.1	

5.3.12.3.5 *Input from level 1a data stream*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*Remarks*
q_{SS}	Stokes fractions (0°/90°) for Rayleigh single scattering	d[R_{FPA}]	-	i	A3.0.4	**MDR-1*-Earthshine** POL_SSQ_POL_SS
u_{SS}	Stokes fractions (–45°/+45°) for Rayleigh single scattering	d[R_{FPA}]	-	i	A3.0.4	**MDR-1*-Earthshine** POL_SSU_POL_SS
$\ddot{q}$	Stokes fractions per PMD band and main channel readout (187.5 ms) for main channel polarisation correction	d[N_{PMD}, 4,R_{FPA}]	-	i	A3.0.4	**MDR-1*Earthshine** POL_MQ_POL
ψ	Scanner viewing angle with additional element at end of scan	d[R_ψ+1]	degree	i	A3.0.4	**MDR_1a*** SCANNER_ANGLE
λ^{MME}	Wavelength grid on which the Müller Matrix Elements will be calculated	d[D,B]	-	i	A3.0.4	**GIADR-1a-MME** MME_WL
$N_{\psi f}$	Number of viewing angles for which the fine viewing angle grid is specified	w	-	i	A3.0.4	**GIADR-1a-MME** MME_N_PSI_F

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
ψ_f	Viewing angles which define the fine viewing angle grid	d[$N_{\psi f}$]	degree	i	A3.0.4	**GIADR-1a-MME** MME_PSI_F
μ^2	Ratio of MMEs M^2 to M^1 describing the polarisation sensitivity of the instrument with respect to the Q Stokes component (s/p polarisation). Derived from key data parameter η.	d[D,B,$N_{\psi f}$]	-	i	A3.0.4	**GIADR-1a-MME** MME_POL_SENS
μ^3	Ratio of MMEs M^3 to M^1 describing the polarisation sensitivity of the instrument with respect to the UStokes component (+/–45° polarisation). Derived from key data parameter ξ.	d[D,B,$N_{\psi f}$]	-	i	A3.0.4	**GIADR-1a-MME** MME_POL_SHIFT
λ_{SS}	Single-scattering wavelength	d[R_{FPA}]	nm	i	A3.0.4	**MDR-1*-Earthshine** POL_SSWL_POL_SS

5.3.12.3.6 Input from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
λ	Wavelength grid of the measurement, FPA and PMD channels.	d[D,B]	nm	i	A3.6	For PMD channels, both the pixel wave-lengths and band wavelengths will be used.
S	Main channel signal from previous correction step.	d[D,B,R_{FPA}]	BU/s	i	A3.9 and various	
E	Absolute error in main channel signal from previous correction step.	d[D,B,R_{FPA}]	BU/s	i	A3.9 and various	

5.3.12.3.7 Output

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
S_{Pol}	Polarisation corrected main channel signal value	d[D,B_{FPA},R_{FPA}]	BU/s	o	A3.11	
E_{Pol}	Absolute error in polarisation corrected main channel signal value	d[D,B_{FPA},R_{FPA}]	BU/s	o	A3.11	
q	Stokes fractions interpolated to main channel detector pixels and main channel timing	d[D,B_{FPA}]	-	o	A3.17.1	**MDR-1b-Earthshine** BAND_MSTOKES_FRACTION

5.3.12.4 Algorithm

Notes:

1. Care must be taken to correctly synchronise main channel signals with PMD channel signals (A3.10.1), single-scattering Stokes fractions, and scanner viewing angles (A3.10.3).
   See Figure 23 in Appendix C. In particular, note that main channel readout n (for $n > 0$) corresponds to single-scattering Stokes fraction $n - 1$, and scanner viewing angle $2n - 1$. The first readout in a scan ($n = 0$) corresponds to single-scattering Stokes fraction $R_{FPA}-1$ in the previous scan, and scanner position $R_{\psi} - 1$ in the previous scan. If there is no information or insufficient information from a previous scan available (because the previous scan is missing or not in one of the earth observation modes) the algorithm cannot be applied for the first readout in the scan. In this case all output parameters for the first readout have to be set to “undefined” and the flag for degraded MDR quality due to a processing degradation (DEGRADED_PROC_MDR) has to be set. The synchronisation with Stokes fractions $\bar{q}$ from PMD averages has been done already instep Calculate Stokes Fractions from PMD Measurements (A2.21.4), so that Stokes fraction $\bar{q}_{imn}$ are the ones to be used for readout n.
2. At this stage, where the measurements of both PMD channels have already been combined into Stokes fractions, the wavelengths of the two PMD channels cannot be treated separately any more. The wavelength grid of PMD p ($j = 5$) is taken here as the reference wavelength grid for both PMDs. This choice is arbitrary. It is assumed that the two PMD channels are co-registered closely enough.

5.3.12.4.1 Establish Time Correlation Between Main Channels and PMD Channels (A3.10.1)

In order to minimise errors in the polarisation correction, a main channel detector pixel signal and the Stokes fraction used for its correction have to correspond as closely as possible to the same ground scene. Therefore the relative timing between the readout of a main channel detector pixel and the readout of a PMD pixel at the same wavelength must be considered. This is determined by the readout time per detector pixel, the readout sequence of the GOME-2 channels (“up” or “down”), and their dispersion relation (pixel – wavelength correspondence).

In processing step *Calculate Stokes Fractions from PMD Measurements* (A2.21.4), four sets of Stokes fractions $\bar{q}$ shifted by one PMD readout (23.4 ms) with respect to each other, have been calculated for each main 187.5 ms channel readout. They are labelled from $m = 0$ to $m = 3$. Here, each main channel detector pixel will be assigned a parameter m^r, expressing its timing relative to the timing of the Stokes fractions. For example, if a pixel has $m^r = 1.6$ (as the one highlighted in Figure 15) it would correspond to a measurement 0.6 × 23.4 ms later then the Stokes fraction from set $m = 1$, and 0.4 × 23.4 ms before Stokes fraction from set $m = 2$. The element m^r will be used in the next step to linearly interpolate between adjacent Stokes fractions for a main channel detector pixel. See Equation 202.

At time origin ($t = 0$), the start of the readout of the main channel is chosen. This corresponds to the start of the last readout of the PMD channels which have been averaged into set $m = 1$ as shown in Figure 15.

Note: To make efficient use of processing time, m^r should be determined only once, and not for every scan. It has to be changed only in the very rare case that the readout sequence is changed. A change in the dispersion relation can safely be neglected.

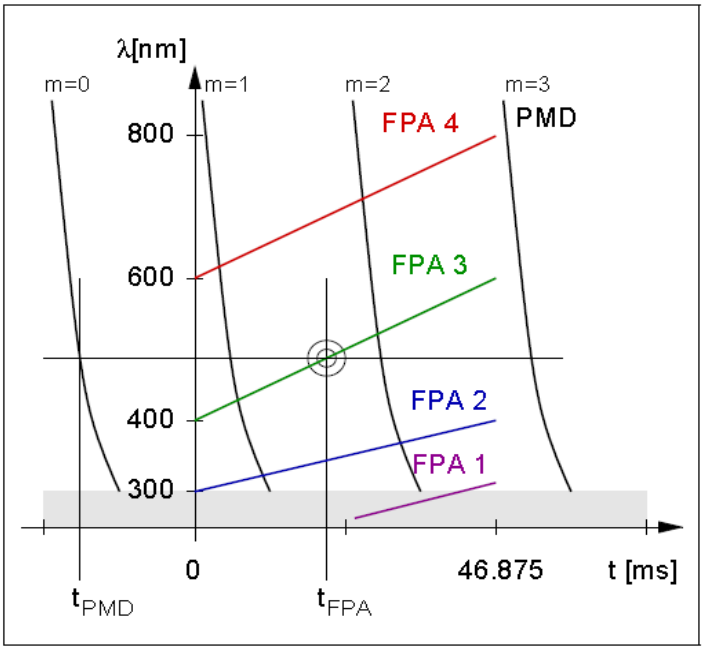

Figure 15: Timing diagram for main channel and PMD detector pixel readouts.
For this example, readout sequence "up" has been assumed for the four main channels, and readout sequence "down" for the two PMD channels. Readout of the main channels and readout of the PMD channels for m = 1 starts att = 0. For a given detector pixel in a main channel, indicated by the circles, its readout time t_{FPA} and the one of the PMD pixel closest in wavelength, t_{PMD} are determined. The difference between the two times is then used for linear interpolation of Stokes fractions between the two adjacent PMD curves.

Loop information: The following calculations are performed for main channels $j = 1\ldots4$, detector pixels $i = 0\ldots D_{FPA} - 1$.

The timing parameters m^r are determined as follows:

Using the PMD p wavelength grid, check whether the main channel wavelength λ_{ij} is within the PMD wavelength range, i.e., whether $\lambda_{ij} \geq \lambda_{768,5}$. ($\lambda_{768,5}$ is the lowest wavelength in PMD p.) If not, (as represented by the shaded area in Figure 15), which is the case for the major part of main channel 1, and possibly a few pixels at the beginning of channel 2, set the following:

$$m_{ij}^r = 0,\ m_{ij}^{r,\text{int}} = 0,\ m_{ij}^{r,\text{frac}} = 0 \quad \text{Equation 196}$$

and we are finished.

Otherwise, determine the time of the readout of detector pixel i in main channel j:

$$t_{\text{FPA}} = \begin{cases} i \cdot \delta_{rd} & \text{(readout sequence up)} \\ (1023 - i) \cdot \delta_{rd} & \text{(readout sequence down)} \end{cases} \quad \text{Equation 197}$$

Using the PMD p wavelength grid, determine the PMD p detector pixel k which is closest in wavelength to the main channel wavelength λ_{ij}.

For this PMD detector pixel k and $m = 0$, determine the time of its readout

$$t_{\mathrm{PMD}} = \begin{cases} (k-768)\cdot\delta_{rd} - 23.4375\cdot 10^{-3} & \text{(readout sequence up)} \\ (1023-k)\cdot\delta_{rd} - 23.4375\cdot 10^{-3} & \text{(readout sequence down)} \end{cases}$$ *Equation 198*

t_{PMD} will be negative.

Calculate the time offset between FPA and PMD measurements (for $m = 0$) in units of 23.4375 ms as follows:

$$m_{ij}^{r} = (t_{\mathrm{FPA}} - t_{\mathrm{PMD}})/(23.4375\cdot 10^{-3})$$ *Equation 199*

Split m_{ij}^{r} into its integer part $m_{ij}^{r,\mathrm{int}}$ and fractional part $m_{ij}^{r,\mathrm{frac}}$, using the C maths library function `modf`.

End of loop.

The following three loops are nested.

Loop 1 information (this loop includes A3.10.2 and A3.10.3): The following calculations are performed for all main channel readouts, i.e., for $n = 0 \ldots R_{\mathrm{FPA}}-1$.

5.3.12.4.2 INTERPOLATE STOKES FRACTIONS TO MAIN CHANNEL WAVELENGTH GRID (A3.10.2)

1. Interpolate the four sets of Stokes fractions to main channel wavelength grid:

Loop 2 information: The following calculations are performed for the four sets of Stokes fractions, i.e., for $m = 0 \ldots 3$.

Starting from the Stokes fractions $q_{\mathrm{SS},n-1}, \bar{q}_{0mn}, \ldots, \bar{q}_{N_{\mathrm{PMD}}-1,mn}$ with associated wavelengths $\lambda_{ss,n-1}, \lambda_{05}, \ldots, \lambda_{N_{\mathrm{PMD}}-1,5}$, exclude the pairs where the Stokes fraction is set to “undefined”. Use the remaining N_v pairs for interpolation to main channel wavelengths as follows.

Loop 3 information: The following calculations are performed for main channels $j = 1 \ldots 4$, detector pixels $i = 0 \ldots D_{\mathrm{FPA}}-1$.

The main channel wavelength range is divided into three wavelength regions, separated by the wavelengths of the first and the last valid Stokes fraction. The Stokes fractions are Akima interpolated in between, and set to the first (last) value otherwise:

Region 1 ($\lambda_{ij} < \lambda_{v,0}$): Set

$$\ddot{q}_{ijm} = q_{v,0}$$ *Equation 200*

Region 2 ($\lambda_{v,0} \le \lambda_{ij} \le \lambda_{v,Nv-1}$):

Determine $\hat{q}_{ijm}$ from the valid Stokes fractions $q_{v,o},\ldots,q_{v,\,Nv-1}$ and their associated wavelengths $\lambda_{v,o},\ldots\ \lambda_{v,\,Nv-1}$ using Akima Interpolation (AX.4) to the wavelength λ_{ij}.

Region 3 ($\lambda_{ij} > \lambda_{v,\,Nv-1}$): Set the following:

$$\hat{q}_{ijm} = q_{v,\,N_v-1} \quad \textit{Equation 201}$$

End of loop 3.

End of loop 2.

2. Reduce the four sets of Stokes fractions $\hat{q}_{ij0}\ldots\hat{q}_{ij3}$ to a single set, taking into account the relative timing m^r between main channels and PMD channels:

$$q_{ij} = (1 - m_{ij}^{r,\,\text{frac}}) \cdot \hat{q}_{ijm} + m_{ij}^{r,\,\text{frac}} \cdot \hat{q}_{ij,\,m+1} \text{ with } m = m_{ij}^{r,\,\text{int}}\ (j = 1\ldots4,\ i = 0\ldots D-1) \quad \textit{Equation 202}$$

5.3.12.4.3 Calculate and Apply Polarisation Correction Factors (A3.10.3)

For all main channel detector pixels ($j = 1\ldots4$, $i = 0\ldots D-1$), interpolate the Müller matrix elements μ^2, μ^3 describing main channel polarisation sensitivity to the scanner viewing angle $\Psi = \psi_{2n-1}$ ($\Psi = \psi_{63}$ of the previous scan for $n = 0$) using Linear Interpolation (AX.2). Then interpolate μ^2 and μ^3 to the wavelength grid of the FPAs also using Linear Interpolation (AX.2). For spectral points outside the wavelength grid of the Müller matrix elements set μ^2 and μ^3 equal to the first (or last) valid value on the original MME wavelength grid.

The interpolated polarisation fractions for each detector pixel can now be used to calculate the polarisation correction factors excluding those readouts where $|q_{SS\,j/8}| < q_{SS,min}$

$$c_{ij} = 1 + q_{ij}\left(\mu_{ij,\,\Psi}^2 + \frac{u_{SS,\,n-1}}{q_{SS,\,n-1}}\mu_{ij,\,\Psi}^3\right) \qquad (j = 1\ldots B_{FPA},\ i = 0\ldots D-1) \quad \textit{Equation 203}$$

For the “C-shape” region where $|q_{SS,\,n-1}| < q_{SS,min}$ the Stokes fraction is calculated as follows:

$$c_{ij} = 1 + q_{ij}\mu_{ij,\,\Psi}^2 + u_{ij}\mu_{ij,\,\Psi}^3 \qquad (j = 1\ldots B_{FPA},\ i = 0\ldots D-1) \quad \textit{Equation 204}$$

where u is determined as follows:

- If $count(where(|q_{SS,\,n-1}| < q_{SS,\,min})) > 2$ calculate both for the forward and backward scan separately the readout indices which bound the “C-shape”, excluding the PMD reset pixels

$$a = min(where(|q_{SS,\,n-1}| < q_{SS,\,min})) - 1 \text{ and} \quad \textit{Equation 205}$$

$$b = max(where(|q_{SS,\,n-1}| < q_{SS,\,min})) + 1 \quad \textit{Equation 206}$$

- Next calculate

$$P_i^a = \sqrt{q_{ia}^2 + \left(\frac{u_{SS,a}}{q_{SS,a}} \cdot q_{ia}\right)^2} \text{ and}$$ *Equation 207*

$$P_i^b = \sqrt{q_{ib}^2 + \left(\frac{u_{SS,b}}{q_{SS,b}} \cdot q_{ib}\right)^2}$$ *Equation 208*

- For $j = a,b$ calculate

$$P_{ij}^x = m_{2j} \cdot \frac{P_i^a}{P_{ss,a}} \cdot P_{ss,j} + m_{1j} \cdot \frac{P_i^b}{P_{ss,b}} \cdot P_{ss,j}$$ *Equation 209*

where $m_2 = 0$ if a does not exist and $m_1 = 0$ if b does not exist and otherwise:

$$m_{1j} = \frac{j-a}{b-a} \text{ and } m_{2j} = \frac{b-j}{b-a}$$ *Equation 210*

- Finally $j = a,b$ for calculate:

$$u_{ij} = P_{ij}^x \cdot \sin 2\chi_{ss,j}$$ *Equation 211*

Notes:

1. Because GOME-2 does not measure the u Stokes component directly, we are assuming the wavelength-independent single-scattering value u_{SS} for u here.
2. In the case that no information from a previous scan is available (e.g., for the first readout of the first scan), c_{ij} is set to "undefined" for all detector pixels i and channels j, and the flag for degraded MDR quality due to a processing degradation (DEGRADED_PROC_MDR) is raised.
3. Single-scattering Stokes fractions and viewing angles should be averaged over the integration time, if longer than 187.5 ms or 93.75 ms respectively.
4. If q_{ij} values are undefined, set c_{ij} to be undefined in these cases.

The following calculations are performed for all main channel readouts: for $n = 0...R_{FPA-1}$.
Main channel signals are polarisation-corrected by dividing them by the polarisation correction factor:

$$S_{Pol,ijn} = S_{ijn}/c_{ij} \qquad (j = 1\ldots B_{FPA}, i = 0\ldots D-1)$$ *Equation 212*

$$E_{Pol,ij} = \sqrt{E_{ij}^2 + (\delta_{pol} \cdot S_{Pol,ijn})^2}$$ *Equation 213*

In the case that c_{ij} is "undefined", set $S_{Pol,ijn}$ and $E_{Pol,ij}$ to "undefined".

End of loop 1.

5.3.13 APPLY RADIANCE RESPONSE (A3.11)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark		FPA	√
Sun		Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon	√		

Uses Generic Sub-Function:

Apply Spectral Calibration (AG.14)

Uses Auxiliary Sub-Functions:

None.

Data Granule

One Scan, with access to the previous scan.

5.3.13.1 Objectives

The application of the radiance response is a division of the detector readouts to be corrected byte MMEs describing the radiance response of the instrument. It is assumed that the main channel signals have been corrected for dark current, normalised to one-second integration time, corrected for PPG, Etalon and stray light, and spectrally calibrated. In the case of the PMDs band mode data are corrected for dark signal only and raw data are corrected for dark signal, PPG and etalon. Both are normalised to 1s integration time. The MMEs describing the radiance response of the instrument (see Section 5.2.3) are calculated for a fixed wavelength grid. Furthermore they are pre-calculated for a fine grid of viewing angles. The MMEs must first be interpolated to the wavelength grid of the measurement to be corrected and to the appropriate viewing angle using Linear Interpolation (AX.2).

PMD signals are treated in two ways in this module: first they are combined into a single “PMD radiance”. This is the most natural approach, as the two PMD channels measure in fact two components of the same signal. Other advantages of this approach compared to calibrating individual PMD channels are as follows:

- Higher signal-to-noise values, and
- Stokes fractions q retrieved in module Apply Polarisation Correction (A3.10) are not required, only the single-scattering Stokes fractions ratio u_{SS}/q_{SS} in case μ^3 is different from 0.

Additionally, independently-calibrated PMD signals without polarisation correction are also provided.

5.3.13.2 Variables

5.3.13.2.1 Local Variables

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
ψ_{meas}	Viewing angle of the measurement (main channel readout)	d	degree	t	-	
Ψ	Viewing angles corresponding to individual PMD readouts, i.e., on 23.4 ms grid. One extra element at the end for convenience.	$d[R_{PMD}+1]$	degree	t	-	A capital Ψ is used to distinguish the variable from the viewing angle ψ on the 93.75 ms grid
$\left.\frac{u}{q}\right\|_{ss}$	Single-scattering Stokes fractions ratio	d	-	t	-	
S^{MME}_{DPE}	Detector readouts for PMDs interpolated onto the wavelength grid of the MMEs.	$d[D,B,R_{PMD}]$	BU/s	t	-	
E^{MME}_{DPE}	Absolute error in detector readouts for PMDs interpolated onto the wavelength grid of the MMEs.	$d[D,B,R_{PMD}]$	BU/s	t	-	
S^{MME}_{Cal}	Detector readouts for PMDs, calibrated but not polarisation corrected, and interpolated onto the wavelength grid of the MMEs.	$d[D,B,R_{PMD}]$	photons/(s.cm^2.sr.nm)	t	-	
E^{MME}_{Cal}	Absolute error in detector readouts for PMDs, calibrated but not polarisation corrected, and interpolated onto the wavelength grid of the MMEs.	$d[D,B,R_{PMD}]$	photons/(s.cm^2.sr.nm)	t	-	
uncorr, $MMES_{Cal}$	Detector readouts for PMDs, calibrated but not polarisation corrected, and interpolated onto the wavelength grid of the MMEs.	$d[D,B,R_{PMD}]$	photons/(s.cm^2.sr.nm)	t	-	

5.3.13.2.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
N_{PMD}	Total number of PMD bands	w	-	i	A3.0.1	
$q_{\mathrm{SS,min}}$	Lower threshold for single-scattering Stokes fraction q_{SS} to avoid singularity in $u_{\mathrm{SS}}/q_{\mathrm{SS}}$	d	-	i	A2.0.1	
SunNorm	Switch indicating whether to store the absolutely calibrated radiance or a sun-normalised radiance with associated errors and PCDs in the level 1b product.	enum	-	i/o	A3.0.1/A3.17.1	**MDR-1b-Earthshine** OUTPUT_SELECTION

5.3.13.2.3 Input from level 1a data stream

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/ Destination*	*Remarks*
λ^{MME}	Wavelength grid for Müller Matrix Elements	d[D,B]	-	i	A3.0.1	**GIADR-1a-MME** MME_WL
$N_{\psi f}$	Number of viewing angles for which the fine viewing angle grid is specified	w	-	i	A3.0.4	**GIADR-1a-MME** MME_N_PSI_F *nominal value 21*
Ψ_f	Viewing angles which define the fine viewing angle grid	d[$N_{\psi f}$]	degree			**GIADR-1a-MME** MME_PSI_F *–50, –45, …, 0, …, 45, 50*
M^1	Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D,B,$N_{\psi f}$]	BU.s^{-1}/(photons/(s.cm^2.sr.nm))	i	A3.0.4	**GIADR-1a-MME** MME_RAD_RESP
ε_M^1	Error in the Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D,B]	BU.s^{-1}/(photons/(s.cm^2.sr.nm))	i	A3.0.4	**GIADR-1a-MME** MME_ERR_RAD_RESP
$\varepsilon\_M^1_{SN}$	Error in the sun-normalised radiance response	d[D,B]	BU.s^{-1}/(photons/(s.cm^2.sr.nm))	i	A3.0.4	**GIADR-1a-MME** MME_SNRR_ERR

Symbol	Descriptive Name	Type	Units	I/O	Source/ Destination	Remarks
μ^2	Ratio of MMEs M^2 to M^1 describing the polarisation sensitivity of the instrument with respect to the Q Stokes component (s/p polarisation).	d[D,B, $N_{\psi f}$]	-	i	A3.0.4	**GIADR-1a-MME** MME_POL_SENS
μ^3	Ratio of MMEs M^3 to M^1 describing the polarisation sensitivity of the instrument with respect to the U Stokes component (+/–45° polarisation).	d[D,B, $N_{\psi f}$]	-	i	A3.0.4	**GIADR-1a-MME** MME_POL_SHIFT
λ^{SMR}	SMR wavelength grid after Doppler correction	d[D,B]	nm	i	A3.0.4	**VIADR-SMR** LAMBDA_SMR
SMR	Solar Mean Reference spectrum	d[D,B]	photons/(s.cm^2.nm)	i	A3.0.4	**VIADR-SMR** SMR
E_{SMR}	Absolute error in the Solar Mean Reference spectrum	d[D,B]	photons/(s.cm^2.nm)	i	A3.0.4	**VIADR-SMR** E_SMR
[illegible]	Relative error in the mean of the N_{sun} solar measurements having passed the intensity and consistency checks, before correction for the irradiance response of the instrument.	d[D,B]	-	i	A3.0.4	**VIADR-SMR** E_REL_SUN
pmd_transfer	PMD transfer mode	enum	-	i	A3.0.4	**MDR-1*** PMD_TRANSFER
ψ	Scanner viewing angles for the complete scan	d[R_{ψ}+1]	degree	i	A3.0.4	**MDR-1a-*** SCANNER_ANGLE
q_{SS}	Stokes fractions (0°/90°) for Rayleigh single-scattering	d[R_{FPA}]	-	i	A3.0.4	**MDR-1*- Earthshine** POL_SSQ_POL_SS
u_{SS}	Stokes fractions (–45°/+45°) for Rayleigh single-scattering	d[R_{FPA}]	-	i	A3.0.4	**MDR-1*-Earthshine** POL_SSU_POL_SS

5.3.13.2.4 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
λ	Wavelength grid of the measurement	d[D,B]	nm	i	A3.6	
S_{DPESP}	Detector readouts for FPAs corrected for dark signal, PPG, Etalon, stray light and polarisation and normalised to an integration time of one second.	d[D,B,R_{FPA}]	BU/s	i	A3.10	
E_{DPESP}	Absolute error in detector readouts for FPAs corrected for dark signal, PPG, Etalon, stray light and polarisation and normalised to an integration time of one second.	d[D,BR_{FPA}]	BU/s	i	A3.10	
S_{DPE}	Detector readouts for PMDs corrected for dark signal, PPG, and Etalon, and normalised to an integration time of one second.	d[D,B,R_{PMD}]	BU/s	i	A3.4 *or* A3.7	*Note that PMD band data are only dark signal corrected and normalised to one-second integration time.*
E_{DPE}	Absolute error in detector readouts for PMDs corrected for dark signal, PPG, and Etalon, and normalised to an integration time of one second.	d[D,BR_{PMD}]	BU/s	i	A3.4 *or* A3.7	*Note that PMD band data are only dark signal corrected and normalised to one-second integration time.*

5.3.13.2.5 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
S_{Cal}	Signal detector readouts corrected for the radiance response of the instrument.	d[D,BR_{FPA}] *or* d[D,BR_{PMD}]	photons/(s.cm^2.sr.nm)	o	A3.17.1 and various	**MDR_1b*** BAND_*RAD
E_{cal}	Absolute error in signal detector readouts corrected for the radiance response of the instrument.	d[D,BR_{FPA}] *or* d[D,BR_{PMD}]	photons/(s.cm^2.sr.nm)	o	A3.17.1 and various	**MDR_1b*** BAND_*ERR_RAD

Symbol	Descriptive Name	Type	Units	I/O	Source/Destination	Remarks
S^{uncorr}_{Cal}	PMD signal detector readouts corrected for the radiance response of the instrument but not polarisation corrected.	d[D,BR$_{PMD}$]	photons/(s.cm^2.sr.nm)	o	A3.17.1 and various	**MDR_1b*** BAND_PUNCORR_RAD
E^{uncorr}_{Cal}	Absolute error in the PMD signal detector readouts corrected for the radiance response of the instrument but not polarisation corrected.	d[D,BR$_{PMD}$]	photons/(s.cm^2.sr.nm)	o	A3.17.1 and various	**MDR_1b*** BAND_PUNCORR_ERR_RAD
R	Sun-normalised radiance or reflectivity.	d[D,BR$_{FPA}$]	-	o	A3.17.1 and various	**MDR_1b*** BAND_*RAD
E_R	Absolute error in sun-normalised radiance or reflectivity.	d[D,BR$_{FPA}$]	-	o	A3.17.1 and various	**225MDR_1b*** BAND_*ERR_RAD

5.3.13.3 Algorithm

Note: Different approaches are used for the radiometric calibration of main channels and PMD channels:

- Main channel signals have been polarisation corrected before (A3.10), and therefore only the absolute radiance response M^1 is applied. For the PMD channels, radiance response M^1 and polarisation responses μ^2, μ^3 are corrected simultaneously. Additionally, PMD data are also provided with radiance response corrected but without polarisation correction.
- PMD channels have shorter integration times. The PMD MMEs have to be interpolated to different (and more) scanner viewing angles than the main channel MMEs.

Therefore, radiometric calibration of main channels and PMD channels is described separately in A3.11.1 and A3.11.2

5.3.13.3.1 Calculate Absolutely Calibrated Radiance for Main Channels (A3.11.1)

Loop information: The calculations below are performed for all main channel readouts in the scan, for $n = 0 \ldots R_{FPA} - 1$.

- Calculate the viewing angle ψ_{meas} from the scanner viewing angles ψ in the level 1a product. The correct scanner viewing angle is given by $\psi_{meas} = \psi_{m(n-½)}$ where m is the ratio of the integration time of the readout to the time increment between scanner angles, i.e. 93.75ms and n is the number of the readout in the scan where the first readout is $n = 0$. Note for $n = 0$ the appropriate scanner viewing angle will be from the previous scan. As in module Apply Polarisation Correction (A3.10), if there is no or insufficient information from a previous scan available (because the previous scan is missing or not in one of the earth observation modes) the algorithm cannot be applied for the first readout in the scan. In this case all output parameters for the first readout have to be set to “undefined” and the flag for degraded MDR quality due to processing degradation (DEGRADED_PROC_MDR) has to be set.
- Interpolate the main channel MMEs M^1 (second dimension $j = 1 \ldots 4$) describing the radiance response of the instrument from the fine viewing angle grid ψ_f to the viewing angle of the measurement ψ_{meas} using Linear Interpolation (AX.2).
- Interpolate the resulting main channel MMEs M^1 and ε_M^1 (second dimension $j = 1 \ldots 4$) describing the radiance response of the instrument at ψ_{meas} from the uniform wavelength grid λ^{MME} to the wavelength grid of the measurement λ using Spline Interpolation (AX.3).
- Calculate the calibrated radiance for all channels $j = 1 \ldots 4$ and all detector pixels $i = 0 \ldots D_j - 1$ as follows:

$$S_{Cal,ijn} = S_{DPESP,ijn} / M^1_{\psi_{meas}}(\lambda_{ij})$$

Equation 214

End of loop.

5.3.13.3.2 CALCULATE ABSOLUTELY CALIBRATED RADIANCE FOR PMD CHANNELS (A3.11.2)

- The description below refers to PMD blocks CDE. For PMD block B set S_{Cal} and E_{Cal} to be "undefined".
- Calculate viewing angles Ψ corresponding to the individual PMD readouts (R_{PMD} + 1 values per scan) from the viewing angles ψ on the 93.75 ms grid of the scanner (R_ψ + 1 values per scan) by linear interpolation as described in Calculate Stokes Fractions from PMD Measurements (A2.21.4), Equations 159 to Equation 161.

Loop information: The calculations below are performed for all PMD readouts in the scan, i.e., for $n = 0 \ldots R_{PMD} - 1$.

- Calculate the single-scattering Stokes fraction ratio $\left.\frac{u}{q}\right|_{SS}$ corresponding to PMD readout n by linear interpolation from the single-scattering Stokes fractions given on the 187.5 ms grid of the main channels:

$$\left.\frac{u}{q}\right|_{SS,n} = \frac{u_{SS,k-1}}{q_{SS,k-1}} + \frac{(n+4)\bmod 8}{8.0}\left(\frac{u_{SS,k}}{q_{SS,k}} - \frac{u_{SS,k-1}}{q_{SS,k-1}}\right) \qquad \text{Equation 215}$$

where $k = (n + 4) / 8$ (integer division) is the index of the first single-scattering Stokes fraction *after* PMD readout n. See Figure 23 in Appendix C. As usual, index –1 refers to index $R_{FPA}-1$ of the previous scan, mod denotes the integer modulo operation, and the division by 8.0 is a float division. For PMD block C (integration time 46.875ms in nominal readout mode) n in Equation 215 and in the expression for k has to be replaced by $n - 1$. If $|q_{SS,k-1}| < q_{SS,min}$ or $|q_{SS,k}| < q_{SS,min}$ the ratio $u_{SS,n} / q_{SS,n}$ in the above equation has to be set to "undefined".

- Interpolate the PMD channel MMEs M^1, μ^2, μ^3 (second dimension $j = s, p$), describing the radiance and polarisation response of the instrument from the fine viewing angle grid ψ_f to the viewing angle of the measurement Ψ_n using Linear Interpolation (AX.2).
- Interpolate the PMD signals S_{DPE} from the wavelength grid of the measurement to the wave-length grid of the MMEs to yield using Linear Interpolation (AX.2).
- Calculate the calibrated PMD radiance for all spectral grid points as follows:

$$S^{MME}_{Cal,in} = \left(\left(\mu^2_{is,\Psi_n} + \mu^3_{is,\Psi_n}\left.\frac{u}{q}\right|_{SS}\right)\frac{S^{MME}_{DPE,ip}}{M^1_{p,\Psi_n}} - \left(\mu^2_{p,i\Psi_n} + \mu^3_{ip,\Psi_n}\left.\frac{u}{q}\right|_{SS}\right)\frac{S^{MME}_{DPE,is}}{M^1_{s,\Psi_n}}\right) / \left(\mu^2_{is,\Psi_n} - \mu^2_{ip,\Psi_n} + (\mu^3_{is,\Psi_n} - \mu^3_{ip,\Psi_n})\left.\frac{u}{q}\right|_{SS}\right) \qquad \text{Equation 216}$$

- Calculate the absolutely-calibrated PMD radiance without polarisation correction for all spectral grid points and $j = p,s$ as follows:

$$S^{uncorr,MME}_{Cal,ijn} = \left(\frac{S^{MME}_{DPE,ij}}{M^{1}_{p,\Psi_n}}\right)$$ *Equation 217*

- Interpolate the calibrated PMD radiances from the MME spectral grid back to the PMDp and PMD s spectral grids to yield $S_{Cal,ipn}$, $S_{cal,isn}$, $S^{uncorr}_{Cal,ipn}$,and $S^{uncorr}_{Cal,isn}$.
- Note that if $\left.\frac{u}{q}\right|_{SS,n}$ is "undefined", $S_{Cal,ipn}$ shall also be set to "undefined".

End of loop.

5.3.13.3.3 CALCULATE THE ACCURACY ON THE CALIBRATED RADIANCES (A3.11.3)

- Calculate the absolute error in the calibrated main channel radiances for $n = 0 \ldots R_{FPA} - 1$, $j = 1 \ldots 4$, $i = 0 \ldots D_j - 1$ as follows:

$$E_{Cal,ijn} = \frac{1}{(M^{1}_{\Psi_{meas}}(\lambda_{ij}))} \cdot \sqrt{E^{2}_{DPESP,ijn} + (\varepsilon\_M^{1}(\lambda_{ij}) \cdot S_{DPESP,ijn})^{2}}$$ *Equation 218*

- Calculate the absolute error in the calibrated PMD radiances (both with and without polarisation correction) for $n = 0 \ldots R_{PMD} - 1$, $j = p,s$, and $i = 0 \ldots D_j - 1$ as follows:

$$E^{MME}_{Cal,ijn} = \frac{1}{(M^{1}_{\Psi_{meas},ij})} \cdot \sqrt{(E^{MME}_{DPE,ijn})^{2} + (\varepsilon\_M^{1}_{ij} \cdot S^{MME}_{DPE,ijn})^{2}}$$ *Equation 219*

- Interpolate the error in the calibrated PMD radiances from the MME spectral grid back to the PMD p and PMD s spectral grids to yield $E_{Cal,ipn}$ and $E_{Cal,isn}$.
- Set $E^{uncorr}_{Cal,ipn} = E_{Cal,ipn}$ and $E^{uncorr}_{Cal,ips} = E_{Cal,isn}$

5.3.13.3.4 CALCULATE THE SUN-NORMALISED RADIANCE (A3.11.4)

- Interpolate the SMR spectrum from its wavelength grid λ^{SMR} to the wavelength grid of the measurement using Spline Interpolation (AX.3).
- If the current PMD transfer mode is *band* while the SMR is only available in *raw* transfer mode, the SMR PMD data has to be converted to *band* transfer mode by co-adding PMD pixels. For the relevant PMD band definition parameters see [AD 9].
- Calculate the sun-normalised radiance or reflectivity for $n = 0 \ldots R_{FPA} - 1$, $j = 1 \ldots B$, $i = 0 \ldots D_j - 1$ as follows:

$$R_{ijn} = \pi \cdot S_{cal,\, ijn} / SMR(\lambda_{ij})$$ *Equation 220*

5.3.13.3.5 CALCULATE THE ACCURACY ON THE SUN-NORMALISED RADIANCE (A3.11.5)

- Calculate the absolute error in the sun-normalised radiance for $n = 0 \ldots R_{FPA}-1$, $j = 1 \ldots B$, $i = 0 \ldots D_j-1$ as follows:

$$E_{R,\, ijn} = R_{ijn} \cdot \sqrt{(E_{DPESP,\, ijn}/S_{DPESP,\, ijn})^2 + (\varepsilon^{BU/s}_{Sun,\, ij})^2 + (\varepsilon\_M^1_{SN,\, ij})^2}$$ *Equation 221*

5.3.14 APPLY IRRADIANCE RESPONSE (A3.12)

Instrument Modes		Instrument Data	
Earth		PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Apply Irradiance Response (AG.18)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.15 CORRECT DOPPLER SHIFT (A3.13)

Instrument Modes		Instrument Data	
Earth		PMD	√
Dark		FPA	√
Sun	√	Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Correct Doppler Shift (AG.19)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan

5.3.16 REDUCE SPATIAL ALIASING (A3.14)

Instrument Modes		Instrument Data	
Earth	√	PMD	√
Dark		FPA	√
Sun		Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Correct Doppler Shift (AG.19)

Uses Auxiliary Sub-Functions:

Spline Interpolation (AX.3)

Data Granule

One scan, with access to the previous scan.

5.3.16.1 Objectives

To correct for the effect of the finite detector pixel readout time which causes individual detector pixels to view slightly shifted ground scenes, an effect referred to as ‘Spatial Aliasing’ as spatial variability is aliased into spectral variability in the measurements.

5.3.16.2 Description

Spatial aliasing is caused by the finite readout time of the main channel and PMD detector pixel arrays. The detector pixels are read out consecutively and therefore each pixel observes a ground scene that is slightly shifted in space. When the ground scene is changing e.g. in the case of cloud/land/water or water/land transitions, the different detector pixels will observe different ground scenes with different spectral signatures. As a result the complete observed spectrum may not be representative of one specific ground scene. Furthermore, since the main channel spectrum is measured using four detector arrays, the resulting spectrum may show spectral jumps between channels due to a different ground scene being observed by the last detector pixels in one channel and the first detector pixels in the next. In this section, a method to correct for these effects is specified.

The principle of the method lies in scaling the main channel detector readouts by the ratio of PMD readouts as they occur during the integration time of the main channels. Since the PMDs have a temporal resolution up to eight times higher than that of the main channels, a representative correction can be obtained by co-adding the PMDs over the integration time of main channel signals and interpolating in time to the exact integration time of each main channel detector pixel. The spatial aliasing correction is calculated for each main channel pixel as the ratio of a reference co-added PMD readout, calculated for the start time of the main channel readout, to the co-added signal, calculated for the time of the pixel readout. The corrections are calculated for a selected PMD band associated with each main channel. The PMD band is chosen to be that closest to a wave-length specified per main channel in the initialisation file. The corrections calculated for the selected PMD bands are finally interpolated to the wavelength of the specific main channel detector pixel to be corrected. Main channel detector readouts with an integration time longer than 1.5 s are not corrected as the spatial aliasing effect will be negligible.

5.3.16.3 Variables

5.3.16.3.1 Indices

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source/Destination*	*Remarks*
k	PMD band index	i	-	t	-	$0\ldots N_{PMD}-1$
l	PMD readout index. If negative, it denotes PMD readout $R_{PMD}+l$ from previous scan.	i	-	t	-	See Equation 223
m	PMD sum index	i	-	t	-	$0\ldots N_{coadd}-1$
n	FPA readout index	i	-	t		$0\ldots R_{FPA}-1$

5.3.16.3.2 Local variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
t^{PMD}_{cent}	Central pixel (may be fractional) for the selected PMD bands	$d[B_{FPA}]$			-	
M	Number of PMD band readouts per main channel readout (i.e., number of PMD readouts to co-add)	$i[B_{FPA}]$		t	-	
t^{FPA}	Timestamps for main channel read-outs relative to first readout of first detector pixel	$d[D,B_{FPA}, R_{FPA}]$	t		-	
t^{PMD}	Timestamps for co-added PMD band readouts relative to first read-out of first detector pixel	$d[B_{FPA}, B_{FPA}, R_{FPA}, N_{coadd}]$		t	-	
$\overline{S}^{PMD}$	Co-added PMD band readouts (at times t^{PMD})	$d[B_{FPA}, B_{FPA}, R_{FPA}, N_{coadd}]$	photons/(s.cm^2.sr.nm) t	t	-	
$\tilde{S}^{PMD}$	Co-added PMD band readouts interpolated to the individual times of the main channel detector pixel readouts (tFPA)	$d[B_{FPA}, D,B_{FPA}, R_{FPA}]$	photons/(s.cm^2.sr.nm)	t	-	
$A(\lambda_k^{PMD})$	Spatial aliasing correction for all detector pixels, main channel bands and main channel readouts, given at wavelength of selected PMD band(one wavelength per main channel)	$d[B_{FPA}, D,B_{FPA}, R_{FPA}]$			-	

t

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$A(\lambda_{ij})$	Spatial aliasing correction for all detector pixels, main channel bands and main channel readouts, interpolated to the wavelengths of the main channel detector pixels	d[D,B_{FPA}, R_{FPA}]			-	

5.3.16.3.3 Input from initialisation dataset

t

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
δ_{rd}	Readout time per detector pixel	d	s	i	A3.0.1	
λ^{alias}	Wavelength to be used for association of a PMD band with each main channel	d[B_{FPA}]	nm	i	A3.0.1	
N_{coadd}	Number of sets of co-added PMD readouts needed to cover the main channel readout time.	i	-		A3.0.1	
λ_{alias}	Four wavelengths used for Akima extrapolation in the "Reduce Spatial Aliasing" algorithm.	d[4]	nm	i	A3.0.1	

i

5.3.16.3.4 Input from level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
mode	Observation mode	enum	-		A3.0.4	**MDR-1** *OBSERVATION_MODE
pmd_transfer	PMD transfer mode	enum	-	i	A3.0.4	**MDR-1** *PMD_TRANSFER
IT	Integration time per band	d[B]	s	i	A3.0.4	**MDR-1** *INTEGRATION_TIMES

i

5.3.16.3.5 Input from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
λ	Wavelength grid of main channel detector readouts	d[D,B_{FPA}]	nm	i	A3.6	
λ^{PMD}	Wavelength grid of PMD band readouts	d[N_{PMD}]	nm	i	A3.6	
S_{cal}	Main channel detector readouts corrected for the radiance response of the instrument.	d[D,B_{FPA}, R_{FPA}]	photons/(s.cm^2.sr.nm)	i	A3.11	
S^{PMD}	PMD band readouts corrected for instrument radiance response	d[N_{PMD},R_{PMD}]	photons/(s.cm^2.sr.nm)	t	A3.11	
S_{cal}^{corr}	Main channel detector readouts corrected for spatial aliasing.	d[D,B_{FPA}, R_{FPA}]	photons/(s.cm^2.sr.nm)	o	A3.17.1	**MDR-1b***BAND_*RAD

5.3.16.4 Algorithm

The spatial aliasing correction is only carried out if Mode is equal to any of the *Earth* observation modes as defined in Section 5.2.5, and *pmd_transfer* = *band* + *mixed* or *band* + *raw*, otherwise nothing is done. A correction can only be calculated for those science data packets where the PMD data is in band mode, otherwise nothing is done. Finally, a spatial aliasing correction is only calculated for those main channel bands with an integration time less than or equal to 1.5 seconds. For longer integration times nothing is done.

Note: Time stamps below are given relative to the first readout (n = 0) of the first main channel detector pixel (i = 0 or i = 1023, depending on the readout sequence), i.e. relative to the time $t_0 + \Delta t_{sm}$ in Figure 23 of Appendix C. The first readout of the first PMD channel detector pixel is assumed to take place at the same time. Spatial aliasing correction will be performed using main channel detector pixel i = 0 (the one at the *short* wavelength end, independent of readout sequence) as a reference, i.e., signals for the other detector pixels which have been observed at different times (earlier or later depending on the readout sequence) will be corrected to the time of pixel i = 0.

5.3.16.4.1 CALCULATE TIME STAMP OF MAIN CHANNEL DETECTOR READOUTS (A3.14.1)

Loop information: The following calculations will be performed for all detector pixels i, all main channels j, and all readouts n in a scan, for $i = 0 \ldots 1023$, $j = 1 \ldots B_{FPA}$, $n = 0 \ldots R_{FPA}-1$.

The time stamp of readout n of detector pixel i in main channel j is calculated depending on the readout sequence of this channel as indicated by ‘Readout Sequence’ in the DSM table (‘normal’= ‘up’ and ‘reverse’ = ‘down’):

$$t_{ijn}^{FPA} = \begin{cases} n \cdot IT_j + i \cdot \delta_{rd} & \text{(readout sequence up)} \\ n \cdot IT_j + (1023 - i) \cdot \delta_{rd} & \text{(readout sequence down)} \end{cases}$$

Equation 222

Note: The maximum number of main channel readouts per Science Data Packet is two, totalling 0.375 seconds (corresponding to an effective integration time of 0.1875 seconds per readout).

Note: Although it is necessary to distinguish main channel bands for specification of integration time, it is the pixel position within the complete main channel array that determines the readout time delay due to the finite readout time of individual detector pixels.

5.3.16.4.2 ASSOCIATE PMD BAND WITH EACH MAIN CHANNEL (A3.14.2)

For each main channel j select a PMD band k_j where $\lambda_{k_j}^{PMD}$ is the PMD band with wavelength nearest to λ_j^{alias}. Only PMD band data from the nominal block D are used.

For the selected PMD bands, determine the central pixel $i_{cent,k}^{PMD}$ as the mean value of the start and end pixel of the band. (For a band containing an even number of pixels, this will be a fractional number.)

5.3.16.4.3 Co-add PMD Readouts (A3.14.3)

The PMD band readouts must be co-added to effective integration times equivalent to those of the main channel readouts to be corrected. For a main channel band integration time *ITj* and PMD integration time IT^{PMD}, $M_j = ITj / IT^{PMD}$ PMD readouts have to be co-added in time. As the readout time per detector pixel is fixed, the readout time for the 256 pixels of a PMD channel is only one quarter of the readout time for the 1024 pixels of a main FPA channel. Consequently, in order to take into account the finite readout time of FPA and PMD channels, $N_{coadd} = 4$ such PMD sums (over M_j PMD readouts each) have to be calculated per main channel integration time, each shifted by one PMD readout with respect to the next. This is completely analogous to the treatment in Determine Stokes Fractions (A2.21), see also Figure 23 in Appendix C which illustrates the synchronisation between FPA and PMD readouts. As in A2.21, the very first FPA integration in a scan coincides with the last PMD readouts of the previous scan, so they have to be accessible here.

Loop information: The following calculations will be performed for all main channel bands *j*, the four selected PMD bands *k*, for all 187.5 ms subpixels *n* of a scan, for all PMD sums *m*, i.e.,

for $j = 1 \ldots B_{FPA}$, $k = k_1 \ldots k_{B_{FPA}}$, $n = 0 \ldots R_{FPA} - 1$, $m = 0 \ldots N_{coadd} - 1$. Co-added PMD band readouts are calculated as follows:

$$\overline{S_{kjnm}^{PMD}} = \sum_{l = M_j(n-1)+m}^{M_j n + m - 1} S_{kl}^{PMD} \qquad \text{Equation 223}$$

where the sum comprises $M_j = IT_j / IT^{PMD}$ PMD readouts. As in A2.21, a negative readout index *l* corresponds to PMD readout RPMD + *l* from the previous scan.

Their time stamps are the ones of the last readout in each sum, calculated for the central detector pixel of the selected band and taking into account the readout sequence of the PMD detectors:

$$t_{kjnm}^{PMD} = \begin{cases} ((M_j n + m - 1) IT^{PMD} + (i_{cent,k}^{PMD} - 768) \cdot \delta_{rd}) & \text{(PMD readout sequence up)} \\ ((M_j n + m - 1) IT^{PMD} + (1023 - i_{cent,k}^{PMD}) \cdot \delta_{rd}) & \text{(PMD readout sequence down)} \end{cases} \qquad \text{Equation 224}$$

End of loop.

5.3.16.4.4 Time Interpolate Co-Added PMD Readouts (A3.14.4)

For $i = 0 \ldots 1023$, $j = 1 \ldots B_{FPA}$, and $k = k_1 \ldots kB_{FPA}$, linearly interpolate the co-added PMD band readouts $\overline{S_{kjnm}^{PMD}}$ from t_{kjnm}^{PDM} to the time stamps of the main channel detector pixel readouts t_{ijn}^{FPS} to yield $\tilde{S}_{kijn}^{PMD}$.

5.3.16.4.5 Calculate Spatial Aliasing Correction per PMD Band (A3.14.5)

In this step, the spatial aliasing correction factor with respect to detector pixel 0 in each main channel, the reference detector pixel, is calculated.

For i = 0…1023, j = 1…B_{FPA}, and k = k_1…$k_{B_{FPA}}$, calculate the spatial aliasing correction at λ_k^{PMD}, the wavelength of PMD band k, as follows:

$$A_{ijn}\left(\lambda_k^{PMD}\right) = \hat{S}_{k0jn}^{PMD} / \hat{S}_{kijn}^{PMD}$$ *Equation 225*

5.3.16.4.6 Wavelength Interpolate Spatial Aliasing Correction (A3.14.6)

Interpolate the spatial aliasing correction $A_{ijn}\left(\lambda_k^{PMD}\right)$ for detector pixel i, main channel band j, and main channel detector readout n from the wavelengths λ_k^{PMD} of the selected PMD bands to the wavelength λ_{ij} associated with the detector pixel to be corrected, using Akima Interpolation (AX.4) to yield $A_{ijn}(\lambda_{ij})$. To ensure correct behaviour of extrapolation for long and short wave-lengths, two virtual alias corrections have to be added on the short wavelength side of PMD band associated with $j = 1$ and the long wavelength side of PMD band associated with $j = B$ respectively, using values provided in λ_{alias}. Akima interpolation then automatically returns constant values at both ends.

5.3.16.4.7 Apply Spatial Aliasing Correction (A3.14.7)

Loop information: The following calculations will be performed for all detector pixels i, all main channels j, and all (completed) readouts n in a scan, i.e., for i = 0…1023, j = 1…B_{FPA}, n = 0…R_{FPA} – 1. Calculate main channel radiances corrected for spatial aliasing as follows:

$$S_{\text{cal}}^{\text{corr}}(\lambda_{ij})_n = S_{\text{cal}}(\lambda_{ij})_n \cdot A_{ijn}(\lambda_{ij})$$ *Equation 226*

End of loop.

5.3.17 CALCULATE FRACTIONAL CLOUD COVER AND CLOUD-TOP PRESSURE (A3.15)

Instrument Modes		Instrument Data	
Earth	√	PMD	
Dark		FPA	√
Sun		Housekeeping	
WLS			
SLS			
SLS over Diffuser			
LED			
Moon			
Other			

Uses Generic Sub-Function:

Correct Doppler Shift (AG.19)

Uses Auxiliary Sub-Functions:

Spline Interpolation (AX.3)

Data Granule

One scan.

5.3.17.1 Objective

To determine an effective fractional cloud cover and cloud top pressure for each GOME-2 ground pixel using main channel detector readouts from in and around the Oxygen-A band.

5.3.17.2 Description

An effective cloud cover and cloud top pressure is retrieved for each GOME-2 ground pixel using the Fast Retrieval Scheme for Clouds from the Oxygen A band (FRESCO), developed by KNMI ([RD 20] and [RD 21]). The continuum absorption in the region of the Oxygen-A band is principally determined by the cloud fraction, the cloud optical thickness (or cloud albedo) and the surface albedo. In the Oxygen-A band itself the reflectivity depends, in addition, on the cloud top pressure since clouds screen most of the oxygen inside and below them. The absorption within the Oxygen-A band is therefore higher for a ground pixel with low cloud than one with high cloud. Combined information on cloud fraction and cloud optical thickness may be derived from the reflectivity in the continuum, and cloud top pressure may be estimated from the depth of the Oxygen-A band. The FRESCO algorithm uses three approximately 1 nm-wide windows around 758 nm (representing continuum and no absorption), 761 nm (strong absorption), and 765 nm (moderate absorption). The FRESCO retrieval method is based on a comparison of measured and simulated reflectivities in these three spectral windows. FRESCO+ is a new version of the FRESCO algorithm, in which single Rayleigh scattering is added in the reflectance database and the retrieval. Rayleigh scattering is mainly important for the almost cloud-free part of the pixels. The FRESCO+ cloud pressure is more reliable than FRESCO for less cloudy scenes, say for effective cloud fractions < 0.15. The FRESCO+ improvement is more relevant for tropospheric trace gas retrievals (like NO_2) than for total O_3 retrieval. The improvements associated with FRESCO+ are also implemented in the GOME-2 operational level 0 to 1b processor [RD23].

5.3.17.3 Variables

5.3.17.3.1 Local Variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
k	Counter variable	i	-	t	-	
R	Reflectivity (for channel 4 only)	d[D]	-	t	-	
E_R	Error in reflectivity (for channel 4 only)	d[D]	-	t	-	
UV	UV albedo as determined from TOMS UV surface Lambertian Equivalent Reflectivity dataset	d	-	t	-	
month	Month of measurements for calculation of *UV* albedo	i	-	t	-	*Range 1...12*
SnowIce	Snow/ice flag	bool	-	t	-	*0 if no snow/ice* *1 if snow/ice*
z_s	Surface height	d	km	t	-	
A_s	Surface albedo	d[N_{ref}]	-	t		*0.02 for sea, modified over land using minimum reflectivity dataset*
θ	Satellite zenith angle at h_0 for the centre of the ground pixel	d	degree	t	-	
θ_0	Solar zenith angle at h_0 for the centre of the ground pixel	d	degree	t	-	
φ	Satellite azimuth angle at h_0 for the centre of the ground pixel	d	degree	t	-	
φ_0	Solar azimuth angle at *h*0 for the centre of the ground pixel	d	degree	t	-	
Δ_φ	Relative azimuth angle between the satellite and the sun at h_0 for the centre of the ground pixel	d	degree	t	-	
$f(\Theta)$	Single-scattering phase function, at h0 (topocentric), for the centre of the ground pixel	d[R_{FPA}]	degree	t	-	
$\alpha_k^{\theta,\theta_0}$	Polynomial coefficients for calculation of transmittance interpolated to the viewing and solar zenith angle, and wavelength grid of the measurements	d[N_{coef}, N_{ref}]	-	t	-	

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
β^{θ,θ_0}	Polynomial coefficients for calculation of Rayleigh single-scattering reflectance interpolated to the viewing and solar zenith angle, and wavelength grid of the measurements	$d[N_{coef}, N_{ref}]$	-	t	-	
R^{meas}	Measured reflectivity or sun-normalised radiance interpolated to the reference wavelength grid to be used for cloud parameter fitting.	$d[N_{ref}]$	-	t	-	
E_R^{meas}	Error in measured reflectivity or sun-normalised radiance interpolated to the reference wavelength grid to be used for cloud parameter fitting.	$d[N_{ref}]$	-	t	-	
σ_R	Standard deviation of reflectivity averaged into wavelength bands comprising errors in both measured and simulated reflectivities	$d[N_{ref}]$	-	t	-	
R^{sim}	Simulated reflectivity	$d[N_{ref}]$	-	t	-	
$\frac{\partial R^{sim}}{\partial_{z_c}}$	Derivative of simulated reflectivity with respect to cloud top height.	$d[N_{ref}]$	-	t	-	*Calculated if SnowIce = 0*
$\frac{\partial R^{sim}}{\partial c}$	Derivative of simulated reflectivity with respect to effective cloud fraction.	$d[N_{ref}]$	-	t	-	*Calculated if SnowIce = 0*
$\frac{\partial R^{sim}}{\partial z}$	Derivative of simulated reflectivity with respect to lower reflecting boundary height, averaged in wave-length bands.	$d[N_{ref}]$	-	t	-	*Calculated if SnowIce = 1*
$\frac{\partial R^{sim}}{\partial A}$	Derivative of simulated reflectivity with respect to lower reflecting boundary albedo.	$d[N_{ref}]$	-	t	-	*Calculated if SnowIce = 1*
z_c	Cloud top height	d	km	t	-	*Calculated if SnowIce = 0*
E_{zc}	Error in cloud top height	d	km	t	-	*Calculated if SnowIce = 0*
z	Lower reflecting surface height	d	km	t	-	*Calculated if SnowIce = 1*
E_z	Error in lower reflecting surface height	d	km	t	-	*Calculated if SnowIce = 1*
χ^2	Chi-square value from fitting iteration	d	km	t	-	
χ^2_{old}	Chi-square value from previous iteration	d	km	t	-	

5.3.17.3.2 *Input from initialisation dataset*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
Δ_{depol}	Depolarisation parameter for Rayleigh scattering	d	-		A3.0.1	
t_{cloud}	Threshold for effective fractional cloud cover	d	-	i	A3.0.1	
t_{UV}	UV albedo threshold for snow/ice	d	-		A3.0.1	
A_c	Lambertian cloud albedo	d	-	i	A3.0.1	
c_{fg}	First guess effective cloud fraction	d	-		A3.0.1	
z_{cfg}	First guess cloud top height	d	km	i	A3.0.1	
A_{fg}	First guess albedo of lower reflecting boundary for retrieval in the presence of snow/ice.	d	-		A3.0.1	
z_{fg}	First guess height of lower reflecting boundary for retrieval in the presence of snow/ice.	d	km	i	A3.0.1	
$\delta\chi^2$	Cut-off for variation in χ^2	d			A3.0.1	
ε_{Rsim}	Relative error in simulated reflectivity	d		i	A3.0.1	
θ_0^{max}	Maximum allowed Solar Zenith Angle	d	degree	i	A3.0.1	
R_{max}	Maximum allowed reflectivity	d	-	i	A3.0.1	
λ_{cont}	Wavelength outside the oxygen-A band representing continuum absorption only	d	-		A3.0.1	
maxiter	Maximum number of iterations for cloud parameter retrieval	d	-	i	A3.0.1	

i

5.3.17.3.3 *Input from static auxiliary dataset*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
NT_{lat}	Number of latitudes in *TOMS* UV Albedo dataset	i	-		A3.0.1	
NT_{lon}	Number of longitudes in *TOMS* UV Albedo dataset	i	-	i	A3.0.1	
T_{lat}	Latitude grid for *TOMS*	$d[NT_{lat}]$	degree	i	A3.0.2	
T_{lon}	Longitude grid for *TOMS*	$d[NT_{lon}]$	degree	i	A3.0.2	
TOMS	*TOMS* UV Surface Lambertian Equivalent Reflectivity dataset	$d[NT_{lat}, NT_{lon},12]$	–	i	A3.0.2	*The dimension twelve refers to month*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
NE_{lat}	Number of latitudes in elevation dataset	i	–	i	A3.0.2	
NE_{lon}	Number of longitudes in elevation dataset	i	–	i	A3.0.2	
E_{lat}	Latitude grid for *Elev*	d[NE_{lat}]	degree	i	A3.0.2	
E_{lon}	Longitude grid for *Elev*	d[NE_{lon}]	degree	i	A3.0.2	
Elev	Elevation	d[NE_{lat}, NE_{lon}]	m	i	A3.0.2	
NR_{lat}	Number of latitudes in minimum reflectivity dataset	i	–	i	A3.0.2	
NR_{lon}	Number of longitudes in minimum reflectivity dataset	i	–	i	A3.0.2	
NR_{λ}	Number of wavelengths in minimum reflectivity dataset	i	–	i	A3.0.2	*nominal value*
λ^R	Wavelength grid for R_{min}	d[NRλ]	nm	i	A3.0.2	*nominal values* *λ = 758 nm and* *λ = 772 nm*
R_{lat}	Latitude grid for R_{min}	d [NR_{lat}]	degree	i	A3.0.2	
R_{lon}	Longitude grid for R_{min}	d[NR_{lon}]	degree	i	A3.0.2	
R_{min}	Minimum reflectivity dataset	d[NR_{λ}, NR_{lat}, NR_{lon}]	-	i	A3.0.2	*from GOME/ERS-2 data approximately 1 x 1 degree resolution*
N_{lev}	Number of atmospheric levels in simulations	i	-		A3.0.2	
z^{stat}	Grid for height of atmospheric layers in simulations	d[N_{lev}]	km	i	A3.0.2	
p^{stat}	Grid for pressure of atmospheric layers in simulations	d[N_{lev}]	hPa i	i	A3.0.2	
N_{coef}	Number of polynomial coefficients for expansion of transmittance	i	-	i	A3.0.2	*nominal value 4*
N_{ref}	Number of wavelengths for which α is parameterised and for cloud parameter fitting.	i	-		A3.0.2	*nominal value 15*
N_{θ}	Number of viewing angles for which α is parameterised	i	-	i	A3.0.2	
N_{θ_0}	Number of solar zenith angles for which α is parameterised	i	-i		A3.0.2	

i

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
λ^{ref}	Wavelength grid for which α is parameterised	$d[N_\lambda]$	nm	i	A3.0.2	
θ^{stat}	Viewing angle grid for which α is parameterised	$d[N_\theta]$	degree	i	A3.0.2	
θ_0^{stat}	Solar zenith angle grid for which α is parameterised	$d[N\theta_0]$	degree	i	A3.0.2	
α	Polynomial coefficients for calculation of transmittance	$d[N_{coef}, N_\lambda, N_\theta, N\theta_0]$	-	i	A3.0.2	
β	Polynomial coefficients for calculation of Rayleigh single-scattering reflectance	$d[N_{coef}, N_\lambda, N_\theta, N\theta_0]$	-		A3.0.2	

5.3.17.3.4 Input from level 1a data stream

i

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
date	Start UTC date/time of the scan	d	fractional days	i	A3.0.4	**MDR-1*** RECORD_HEADER RECORD_START_TIME

5.3.17.3.5 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
alon	Geocentric longitude corresponding to actual integration time, ground, points ABCDF (earth-fixed CS)	$d[R_{FPA},5]$	degree	i	A3.2	
alat	Geodetic latitude corresponding to actual integration time, ground, points ABCDF (earth-fixed CS)	$d[R_{FPA},5]$	degree	i	A3.2	
φ_{aSun}	Solar azimuth corresponding to actual integration time, h_0, EFG (topocentric CS)	$d[R_{FPA},3]$	degree	o	A3.2	
θ_{aSun}	Solar zenith corresponding to actual integration time, h_0, EFG (topocentric CS)	$d[R_{FPA},3]$	degree	o	A3.2	
φ_{aSat}	Satellite azimuth corresponding to actual integration time, h_0, EFG (topocentric CS)	$d[R_{FPA},3]$	degree	o	A3.2	
λ	Wavelength grid of the measurements (from channel 4 only)	$d[R_{FPA},D]$	nm	i	A3.6	
R^{sun}	Sun-normalised radiance (from channel 4 only)	$d[R_{FPA},D]$	-	i	A3.14	
ε_R^{sun}	Error in sun-normalised radiance(from channel 4 only)	$d[R_{FPA},D]$	-	i	A3.14	

5.3.17.3.6 Global PCDs accumulated per product

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{cloud}	Number of scans with fractional cloud above a specified threshold	w	-	g	A3.16	

5.3.17.3.7 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$FitMode$	Flag indicating cloud fitting mode	enum	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDFIT_MODE
$CloudFail$	Fail flag for cloud parameter fitting	enum	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDFAIL_FLAG
p_c	Cloud top pressure	d	hPa	o	A3.17.1	**MDR-1b-Earthshine** CLOUDFIT_1 *calculated if SnowIce = 0*
c	Effective cloud fraction	d	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDFIT_2 *calculated if SnowIce = 0*
E_{pc}	Error in cloud top pressure	d	hPa	o	A3.17.1	**MDR-1b-Earthshine** CLOUDE_FIT_1 *calculated if SnowIce = 0*
E_c	Error in effective cloud fraction	d	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDE_FIT_2 *calculated if SnowIce = 0*
p	Lower reflecting surface pressure	d	hPa	o	A3.17.1	**MDR-1b-Earthshine** CLOUDFIT_1 *calculated if SnowIce = 1*
A	Albedo for lower reflecting surface	d	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDFIT_2 *calculated if SnowIce = 1*
E_p	Error in lower reflecting surface pressure	d	hPa	o	A3.17.1	**MDR-1b-Earthshine** CLOUDE_FIT_1 *calculated if SnowIce = 1*
E_A	Error in albedo for lower reflecting surface	d	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDE_FIT_2 *calculated if SnowIce = 1*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$Cloud_{gof}$	Final chi-square goodness of fit after fitting cloud parameters	d	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDGOOD_FIT
$\delta\chi^{2,final}$	Final chi-square perturbation after fitting cloud parameters	d	-	o	A3.17.1	**MDR-1b-Earthshine** CLOUDFINAL_CHI_SQUARE
F_{cloud}	Flag indicating whether effective fractional cloud is greater than a specified threshold	bool	-	o	A3.17.1	**MDR-1b-Earthshine** PCD_EARTH_1BF_CLOUD *1 = above threshold* *0 = below threshold*

5.3.17.4 Algorithm

The following calculations shall only be performed if $\theta_0 < \theta_0^{max}$. Otherwise the output cloud parameters shall be set to “undefined”.

5.3.17.4.1 WAVELENGTH INTERPOLATE MEASURED REFLECTIVITIES (A3.15.1)

- If the sun normalised radiance has not been selected in Apply Radiance Response (A3.11) calculate it as specified therein.
- Calculate the reflectance and the error in the reflectance as $R = R^{sun}/\cos(\theta_0)$ and $E_R = E_R^{sun}/\cos(\theta_0)$ respectively.
- Interpolate the measured reflectivities and their absolute errors from the wavelength grid of the measurement λ to the wavelength grid of the reference simulations λ^{ref} using Spline Interpolation (AX.3) to yield R^{meas} and E_R^{meas} .
- Then if $A_c < R^{meas}(\lambda_{cont}) < R_{max}$ then set $A_c = R^{meas}(\lambda_{cont})$
- A_c is written to **MDR-1b-Earthshine** CLOUD CLOUD_ALBEDO

5.3.17.4.2 INTERPOLATE STATIC AUXILIARY DATA (A3.15.2)

5.3.17.4.2.1 TOMS UV Albedo (A3.15.2.1)

- Calculate the month for which the measurement data is valid (*month*) from the UTC date/time of the measurement.
- Calculate the UV albedo *UV* for the measurement latitude (*lat*) and longitude (*lon*) by Spline Interpolation (AX.3) of TOMS from the grids T_{lat} and T_{lon} for month.
- If $UV > t_{UV}$ then $SnowIce = 1$ else $SnowIce = 0$.
- If UV is undefined in the database set $UV = 1$ and $SnowIce = 1$.

5.3.17.4.2.2 Surface Height (A3.15.2.2)

- Calculate the surface height z_s for the measurement latitude (*lat*) and longitude (*lon*) by Spline Interpolation (AX.3) of *Elev* from the grids E_{lat} and E_{lon}.

5.3.17.4.2.3 Surface Albedo (A3.15.2.3)

If $SnowIce = 0$ then calculate the wavelength-dependent surface albedo as follows. If $SnowIce = 1$ then the distinction between surface and cloud albedo is not made and A_s is not required.

- Calculate the minimum reflectivity $R_{min}(lat, lon)$ for the measurement latitude (*lat*) and longitude (*lon*) by Spline Interpolation (AX.3) of R_{min} from the grids R_{lat} and R_{lon}.
- Subsequently for *i* for $i = 1...N_{ref}$ calculate by Spline Interpolation (AX.3) of $R_{min}(lat,lon)$ between λ_{R1} and λ_{R2}.
- If $R_{min}(\lambda_{R1}) \geq A_c$ then also set $SnowIce = 1$
- A_s is written to **MDR-1b-Earthshine** CLOUD SURFACE_ALBEDO

5.3.17.4.2.4 Polynomial Coefficients (A3.15.2.4)

- Calculate the appropriate solar zenith angle θ_0 , satellite zenith angle θ, solar azimuth angle φ_0 and satellite azimuth angle φ from the set of basic geolocation parameters calculated in Calculate Geolocation for Actual Integration Times (A3.2) θ_{aSun}, θ_{aSat}, φ_{aSun} and φ_{aSat}. For each readout the angles appropriate to the middle of the integration time should be selected.
- Interpolate the polynomial coefficients for calculation of transmittance α from the viewing angle and solar zenith angle grids θ^{ref} and θ_0^{ref} of the reference data, to the satellite zenith angle and the solar zenith angle of the measurement, θ and θ_0 , using 'Spline Interpolation (AX.3)' to yield α^{θ,θ_0}.
- Interpolate the polynomial coefficients for calculation of Rayleigh single-scattering reflectance from the viewing angle and solar zenith angle grids θ^{ref} and θ_0^{ref} of the reference data, to the satellite zenith angle and the solar zenith angle of the measurement, θ and θ_0 , using Spline Interpolation (AX.3)' to yield β^{θ,θ_0}.
- Determine the single-scattering phase function f(Θ) per readout of main channel band 4 data as follows:
  - Calculate the relative azimuth angle $\Delta\varphi = 360 - (\varphi - \varphi_0)$.
  - The cloud fitting algorithm follows the relative azimuth convention as follows: if $\Delta\varphi > 180$, set $\Delta\varphi = \Delta\varphi - 180$.
  - Calculate the cosine of the single-scattering angle as follows:

$$\cos\Theta = -\cos\theta_{Sat}\cos\theta_{Sun} + \sin\theta_{Sat}\sin\theta_{Sun}\cos(\Delta\varphi)$$ *Equation 227*

Calculate the single scattering phase function as: *Equation 228*

$$f(\Theta) = \frac{1}{4\cos(\theta_0)} \cdot \frac{3(1-\Delta_{depol})}{4(1-\Delta_{depol}/2)} \cdot \left((\cos\Theta)^2 + \frac{(1+\Delta_{depol})}{(1-\Delta_{depol})}\right)$$ *Equation 229*

5.3.17.4.3 Calculate Simulated Reflectivities for Fitting (A3.15.3)

If *SnowIce* = 0 then calculate the simulated reflectivity and derivatives as follows:

- Calculate the simulated reflectivity R^{sim} for $i = 1...N_{ref}$ as follows:

$$R_i^{sim} = A_c \cdot c \cdot \left(\sum_{p=0}^{N-1} \alpha_p^{\theta,\theta_0}(\lambda_i^{ref}) \cdot z_c^p\right) + A_s(\lambda_i^{ref}) \cdot (1-c) \cdot \left(\sum_{p=0}^{N-1} \alpha_p^{\theta,\theta_0}(\lambda_i^{ref}) \cdot z_s^p\right) + f(\Theta) \cdot c \cdot \left(\sum_{p=0}^{N-1} \beta_p^{\theta,\theta_0}(\lambda_i^{ref}) \cdot z_c^p\right) + f(\Theta) \cdot (1-c) \cdot \left(\sum_{p=0}^{N-1} \beta_p^{\theta,\theta_0}(\lambda_i^{ref}) \cdot z_s^p\right)$$ *Equation 230*

- Calculate the derivative of R^{sim} with respect to c and z_c for $i = 1...N_{ref}$ as:

$$\frac{\partial R_i^{sim}}{\partial c} = A_c \cdot \left(\sum_{p=0}^{N-1} \alpha_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_c^p\right) - A_s(\lambda_i^{ref}) \cdot \left(\sum_{p=0}^{N-1} \alpha_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_s^p\right) \quad \text{and}$$
$$+ f(\Theta) \cdot \left(\sum^{N-1} \beta_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_c^p\right) + f(\Theta) \cdot \left(\sum^{N-1} \beta_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_s^p\right)$$

Equation 231

$$\frac{\partial R_i^{sim}}{\partial z_c} = A_c \cdot c \cdot \sum_{p=0}^{N-1} p \cdot \alpha_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_c^{p-1} + f(\Theta) \cdot c \cdot \left(\sum_{p=0}^{N-1} \beta_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_c^p\right)$$

Equation 232

If *SnowIce* = 1 then calculate the simulated reflectivity and derivatives as follows:

- Calculate the simulated reflectivity R^{sim} for $i = 1...N_{ref}$ as:

$$R_i^{sim} = A \cdot \left(\sum_{p=0}^{N-1} \alpha_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z^p\right) + f(\Theta) \cdot \left(\sum_{p=0}^{N-1} \beta_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_c^p\right)$$

Equation 233

- Calculate the derivative of R^{sim} with respect to A and z for $i = 1...N_{ref}$ as:

$$\frac{\partial R_i^{sim}}{\partial A} = \left(\sum_{p=0}^{N-1} \alpha_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z^p\right) \quad \text{and}$$

Equation 234

$$\frac{\partial R_i^{sim}}{\partial z} = A \sum_{p=0}^{N-1} p \cdot \alpha_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z^{p-1} + f(\Theta) \cdot \left(\sum_{p=0}^{N-1} \beta_p^{\theta, \theta_0}(\lambda_i^{ref}) \cdot z_c^{p-1}\right)$$

Equation 235

- Calculate the combined error in the measured and simulated reflectivities for $k = 1...N_{ref}$ as:

$$\sigma_{R,i} = \sqrt{(E_{R,i}^{meas})^2 + (\varepsilon_{Rsim} \cdot R_i^{sim})^2}$$

Equation 236

5.3.17.4.4 Cloud Parameter Fitting (A3.15.4)

The cloud parameter fitting is carried out using the Levenberg-Marquardt method as described on page 678 in [RD 10].

1. First call "mrqmin" with the following input parameters:
   - Linearisation point for minimisation defined by λ_{ref} (referred to as vector *x* in [RD 10] and required as input to *funcs*)
   - Measured band reflectivities R^{meas} at linearisation point (referred to as vector y in [RD 10])
   - Standard deviation of the data points σ_R (referred to as matrix *sig* in [RD 10])
   - Number of data points N_{ref} (referred to as *ndata* in [RD 10])
   - Input parameters both static and those to be fitted where the values of parameters to be fitted are set to the "first guess" value for the first iteration.

     If $SnowIce = 0$ then $Param = [z_{cfg}, c_{fg}, A_c, z_s, A_s(\lambda), \alpha^{\theta,\theta_0}(\lambda), \beta^{\theta,\theta_0}(\lambda), f(\Theta)]$ and

     if $SnowIce = 1$ then $Param = [z_{fg}, A_{fg}, \alpha^{\theta,\theta_0}(\lambda), \beta^{\theta,\theta_0}(\lambda), f(\Theta)]$

     (referred to as vector *a* in [RD10] and required as input to *funcs*)
   - Mask indicating which parameters are static and which are fitted.
     If *SnowIce* = 0 then *FitMask* = [1,1,0,0,0,0,0,0] and
     if *SnowIce* = 1 then *FitMask* = [1,1,0,0,0] where 1 indicates the parameter is to be fitted and 0 that it is not to be fitted (referred to as vector *ia* in [RD10]).
   - Total number of parameters N_{param} (referred to as *ma* in [RD10])
   - Arrays to be used as working space and to return output values *Work1* and *Work2* (referred to as matrices covar and alpha in [RD10])
   - Dimension of arrays to be used as working space N_{work} (referred to as *nca* in [RD 10])
   - The Chi-square variable χ^2 to be used in the minimisation (referred to as *chisq* in [RD 10]
   - The function which determines the relationship between the input parameters λ_{ref} and *Param*,

     and the simulated reflectivities R^{sim} with derivatives, if *SnowIce = 0,* $\frac{\partial R^{sim}}{\partial c}$ and $\frac{\partial R^{sim}}{\partial z_c}$, and if *SnowIce* = 1, $\frac{\partial R^{sim}}{\partial A}$ and $\frac{\partial R^{sim}}{\partial z}$. Note that derivatives are only required for those parameters which are to be fitted. This function is described in A3.15.3 above (referred to as *funcs* in [RD10]).
   - Parameter l_a is supplied as input and is set to $l_a < 0$ on the initial call (referred to as *alamda* in [RD 10])

2. Check whether the fitted parameters have physically reasonable values and if not reset as follows:

   - If *SnowIce = 0* then if $z_c < 0$ set $z_c = z_s$ or if $z_c > 15$ set $z_c = 15$. Similarly if $c < –0.05$ set $c = 1e^{-5}$(avoid zero since in this case the derivative becomes zero) or if $c > 1.1$ set $c = 1$.

   - Similarly if *SnowIce = 1* then if $z < 0$ set $z = 0$ or if $z > 60$ set $z = 60$. Similarly, if $A < -0.05$ set $A = 0$ or if $A > R_{max}$ set $A = R_{max}$.

   - In the case that the fitted parameters have been reset, also recalculate the derivatives as described above.

3. Store the value of χ^2 as χ^2_{old} and repeat the call to “mrqmin” using the values of l_a and *Param* output from the previous iteration as input to this iteration.

4. Convergence has been achieved if $0 < \chi^2_{old} - \chi^2 < \delta\chi^2$

5. Repeat Step 2 until convergence has been reached or until *niter* = *maxiter*.

6. Call “mrqmin” one last time with $l_a = 0$ to obtain the final estimate if *SnowIce* = 0 of Param = [z_c, c, A_c, z_s, $A_s(\lambda)$, $\alpha^{\theta, \theta0}(\lambda)$, $\beta(\lambda)$]where the relevant fitted parameters are z_c and c and if *SnowIce* = 1 of where the relevant fitted parameters are z and A.

7. The final result for the cloud fraction c is set to “0” in the case $c < 0$. Values for $c > 1$ are kept (for use in solar radiation applications, see [RD23] Section 4.6).

8. The error covariance of the fitted parameters is returned in *Work1*(*1*: N_{param},*1*: N_{param}) and their curvature in *Work2*(*1:* N_{param},*1:* N_{param}). Parameters which are held fixed will return zero covariance and curvature values. Therefore if *SnowIce* = 0 then $E_{ZC} = \sqrt{Work(1, 1)}$ and $E_C = \sqrt{Work(2, 2)}$, and if *SnowIce* = 1 then $E_Z = \sqrt{Work(1, 1)}$ and $E_A = \sqrt{Work(2, 2)}$

5.3.17.4.5 CONVERT HEIGHT (KM) TO PRESSURE (hPa) (A3.15.5)

- Calculate the cloud top pressure pc or the lower reflecting boundary pressure p as appropriate by ‘Linear Interpolation (AX.2)’ of z_c or z from z^{stat} to p^{stat}
- If $z_c – E_{zc} < 0$ set $z_c – E_{zc} = 0$ or if $z_c + E_{zc} > 60$ then set $(z_c + E_{zc}) = 60$.
- Calculate the error of the cloud top pressure E_{pc} as appropriate as $E_{pc} = max(|p_c - p(z_c - E_{zc})|, |p_c - p(z_c + E_{zc})|)$ where $p(z_c - E_{zc})$ and $p(z_c + E_{zc})$ are calculated by “Linear Interpolation (AX.2)’ of $z_c \pm E_{zc}$ from z^{stat} to p^{stat}. Alternatively, calculate the error in the lower reflecting boundary pressure E_p as appropriate as $E_p = max(|p - p(z - E_z)|, |p - p(z + E_z)|)$ where $p(z - E_z)$ and $p(z + E_z)$ are calculated by ‘Linear Interpretation (AX.2)’ of $z \pm E_z$ from z^{stat} to p^{stat}.
- If $p_c < 130$ hPa set $p_c = 130$ hPa and if $p_c > 1013$ hPa set $p_c = 1013$ hPa.
- In the same manner the surface pressure is calculated from z_s and written to **MDR-1b-Earth-shine C**LOUD SURFACE_PRESSURE.

5.3.17.4.6 CALCULATE PCDs FROM CLOUD PARAMETERS (A3.15.6)

- *CloudFail* is initialised to *success*, and F_{cloud} is initialised to zero.
- *Fitmode = SnowIce*
- If $R_i > R_{max}$ or $R_i < 0$, or $R_k^{sim} > R_{max}$ or $R^{sim} < 0$, for any $i = 1 \ldots N_{ref}$ and any iteration set *CloudFail = reflectivity_out_of_range*
- If $\theta_0 > \theta_0^{max}$ or $\theta_0 < 0$ then set *CloudFail = solar_zenith_out_of_range*
- If $\theta < \theta^{ref}(1)$ or $\theta < \theta^{ref}(N_\theta)$ then set *CloudFail = satellite_zenith_out_of_range*
- If the fitting has not converged and the number of iterations is greater than *maxiter* set *CloudFail = no_convergence*
- If any input data specified above is missing set *CloudFail = missing_input*
- $Cloud_{gof} = gammq((nref - 2.0)/2.0, \chi^2/2.0)$ for final iteration where the incomplete gamma function routine `gammq` is described in [RD9] for final iteration.
- If *SnowIce = 0* and if c > t_{cloud} then set F_{cloud} = 1 and $N_{cloud} = N_{cloud} + 1$ otherwise $F_{cloud} = 0$

5.3.18 COLLECT GLOBAL PCDs PER PRODUCT (A3.16)

Uses Generic Sub-Function:

Correct Doppler Shift (AG.19)

Uses Auxiliary Sub-Functions:

Spline Interpolation (AX.3)

Data Granule

One product assumed to be ‘dump to dump’.

5.3.18.1 Objective

To collect all global PCDs at the completion of processing of one complete product, assumed in this context to be ‘dump to dump’, including those written to the level 1a product. The PQE functionality will also make use of these global PCDs.

5.3.18.2 Description

All global PCDs, indicated in the variable tables by the type ‘g’, are collected at the completion of processing of one complete product, assumed in this context to be ‘dump to dump’. Global PCDs are typically flags indicating non-nominal behaviour and cumulative counts of the number of occurrences of non-nominal behaviour. Information describing observation mode statistics is also included. All global PCDs included in the level 1a product are also included in the level 1b product.

5.3.18.3 Variables

5.3.18.3.1 Global PCDs per product

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
N_{scan}	Number of scans in the product	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_SCANS
N_{val_dp}	Number of valid scans with missing data packets	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_VALID_WITH_MISS_DP
N_{miss_dp}	Number of missing data packets invalid scans	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_MISS_DP
N_{val_dp}	Number of valid scans with missing data packets	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_VALID_WITH_MISS_DP
N_{miss_scan}	Number of missing scans	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_MISSING_SCANS
N_{nn_dt}	Number of scans with non-nominal detector temperature	w[B]	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NN_DETECTOR_TEMP
N_{nn_pdp}	Number of scans with non-nominal pre-disperser prism temperature	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NN_PDP_TEMP
N_{nn_rad}	Number of scans with non-nominal radiator temperature	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NN_RAD_TEMP
N_{nn_WLSU}	Number of scans with non-nominal WLS lamp voltage	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NN_WLS_U
N_{nn_WLSI}	Number of scans with non-nominal WLS lamp current	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NN_WLS_I
N_{nn_SLSU}	Number of scans with non-nominal SLS lamp voltage	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NN_SLS_U
N_{nn_SLSI}	Number of scans with non-nominal SLS lamp current	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NN_WLS_I

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
N_{inv_UTC}	Number of scans with invalid UTC	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_INV_UTC
N_{Nad_scan}	Number of scans in *Nadir_scan* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NADIR_SCAN
N_{Nth_scan}	Number of scans in *Nth_pole_scan* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NTH_POLE_SCAN
N_{Sth_scan}	Number of scans in *Sth_pole_scan* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_STH_POLE_SCAN
N_{Oth_scan}	Number of scans in *Other_scan* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_OTHER_SCAN
N_{Nad_static}	Number of scans in *Nadir_static* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_NADIR_STATIC
N_{Oth_static}	Number of scans in *Other_static* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_OTHER_STATIC
N_{Dark}	Number of scans in *Dark* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_DARK
N_{LED}	Number of scans in *LED* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_LED
N_{WLS}	Number of scans in *WLS* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_WLS
N_{SLS}	Number of scans in *SLS* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_SLS
N_{SLS_diff}	Number of scans in *SLS* over diffuser observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_SLS_DIFF
N_{Sun}	Number of scans in *Sun* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_SUN
N_{Moon}	Number of scans in *Moon* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_MOON

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{Idle}	Number of scans in *Idle* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_IDLE
N_{Test}	Number of scans in *Test* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_TEST
N_{Dump}	Number of scans in *Dump* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_DUMP
$N_{Invalid}$	Number of scans assigned an *Invalid* observation mode	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_INVALID
N_{sat}	Number of scans with saturated pixels	w[B]	-	g/o	A3.0.4/A3.17.3	**SPHR** N_SATURATED
N_{hot}	Number of scans with hot pixels	w[B]	-	g/o	A3.0.4/A3.17.3	**SPHR** N_HOT
N_{min}	Number of scans where the mean uncalibrated signal is below a specified threshold per band	w[B]	-	g/o	A3.0.4/A3.17.3	**SPHR** N_MIN_INTENSITY
N_{SAA}	Number of scans in the SAA	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_SAA
$N_{sunglint}$	Number of scans with sunglint danger	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_SUNGLINT
$N_{rainbow}$	Number of scans with rainbow danger	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_RAINBOW
$N_{mode,geo}$	Number of scans with possible mismatch between observation mode and geolocation	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_MODE_GEOLOCATION
$N_{\mathrm{MissStokes}}$	Number of scans with missing Stokes fractions	w[N_{PMD}]	-	g/o	A3.0.4/A3.17.3	**SPHR** N_MISS_STOKES
$N_{\mathrm{BadStokes}}$	Number of scans with bad Stokes fractions	w[N_{PMD}]	-	g/o	A3.0.4/A3.17.3	**SPHR** N_BAD_STOKES
N_{cloud}	Number of scans with fractional cloud above a specified threshold	w	-	g/o	A3.0.4/A3.17.3	**SPHR** N_CLOUD

5.3.18.4 WRITE LEVEL 1B PRODUCT (A3.17)

Uses Generic Sub-Function:

None.

Uses Auxiliary Sub-Functions:

None.

Data Granule

One product assumed to be ‘dump to dump’.

5.3.18.5 Objective

To collate and write all information to be written to the level 1b product as specified in [AD 4] and [AD 5].

5.3.18.6 Description

All information to be included in the level 1b product is collated and formatted as specified in [AD 4] and [AD 5]. Specific references to fields contained within [AD 4] and [AD 5] are included in the variable tables in this chapter.

5.3.18.7 Variables

As defined in [AD 4] and [AD 5] and referenced previously in variable tables.

5.3.18.8 Algorithm

5.3.18.8.1 Generate level 1b measurement data records (A3.17.1)

The level 1b data records consist of the contents of the MDR-1b data records as specified in [AD 4] and [AD 5].

5.3.18.8.2 Generate in-flight calibration data (A3.17.2)

The in-flight data records consist of the contents of the VIADR-1b-* data records specified in [AD 4] and [AD 5]. These records should contain the same data as those included in the equivalent level 1a product.

5.3.18.8.3 Generate header and global product information (A3.17.3)

The header and global product information consists of the MPHR, SPHR, GEADR-*, and GIADR-* and data records specified in [AD 4] and [AD 5]. For the band start/end wavelengths in GIADR-1b-Bands, the wavelength calibration information corresponding to the last scan of the product has to be used.

5.4 Sensor Performance Assessment (SPA) (A4)

5.4.1 Processing Overview

The Sensor Performance Assessment (SPA) functionality shall allow instrument performance to be monitored for the lifetime of the mission. Performance shall be monitored both from an engineering point of view, utilising selected housekeeping data, and from a scientific point of view utilising spectral data, in particular in-flight calibration data. The SPA functionality comprises extraction, preprocessing and analysis of the monitoring parameters. From the analysis, degradation correction factors (m-factors) shall be derived. The monitoring parameters shall be stored in an SPA data storage location for the lifetime of the mission.

The SPA consists of two building blocks:

1. Monitoring data are extracted from level 1a products, level 1b products, and in-flight calibration datasets. They are preprocessed and written to the SPA data storage location. This is done on a per product basis, as soon as the products and in-flight calibration data are available.
2. Monitoring data for a given timeframe are retrieved from the SPA data storage location and further analysed. Degradation correction factors are calculated where appropriate. This is done offline at regular intervals.

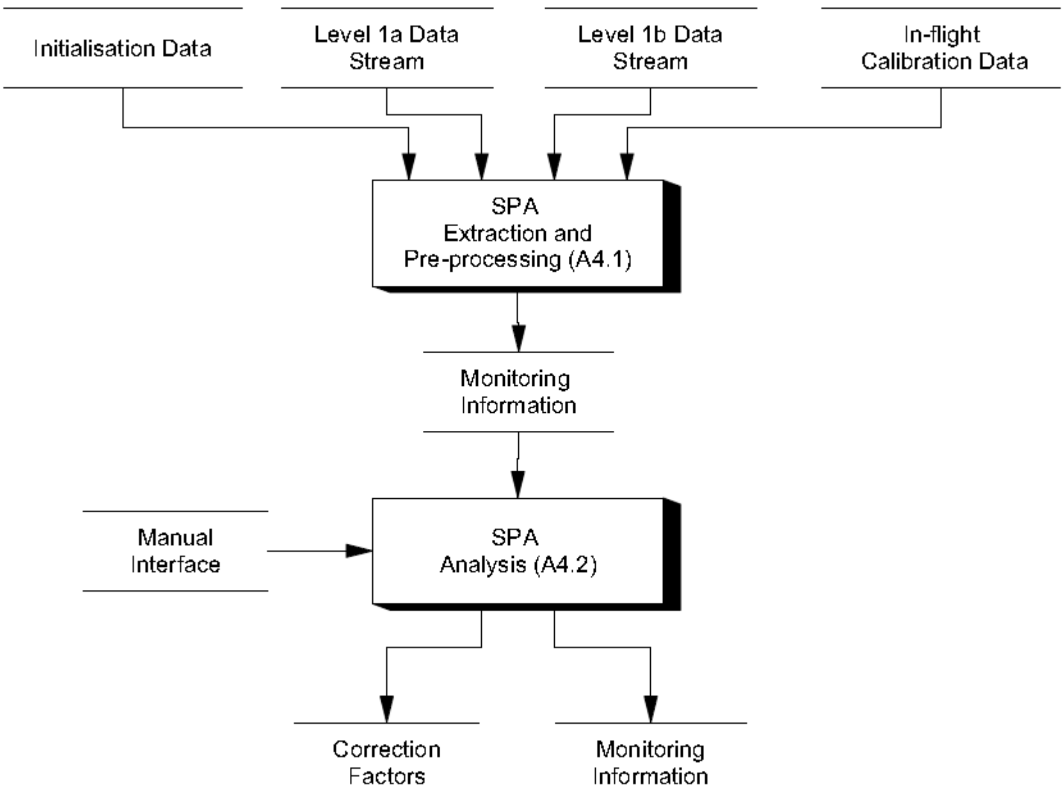

Figure 16: A4 Functional Decomposition: SPA functionality.

5.4.2 SPA EXTRACTION AND PRE-PROCESSING (A4.1)

Input:

Level 1a products.

Level 1b products.

In-flight calibration datasets.

Output:

Preprocessed monitoring information to SPA data storage location.

Uses Generic Sub-functions

Convert Housekeeping Data (AG.4)

Uses Auxiliary Sub-functions:

None.

Data Granule:

None.

Uses Generic Sub-functions

One product or one or more in-flight calibration datasets.

5.4.2.1 Objectives

To extract monitoring information from the level 1a and 1b data products and the in-flight calibration datasets, preprocess them, and write to the SPA data storage location.

5.4.2.2 Description

Monitoring information consists of housekeeping data and spectral data, along with their respective time-tags and geolocation information. Housekeeping data and selected calibration and earth-shine spectral data are extracted from the level 1 products. In-flight calibration data are extracted from in-flight calibration datasets. Housekeeping data are converted from binary units to physical units and condensed into mean, minimum, maximum and standard deviation values per scan. Spectral data are preprocessed according to the instrument mode. All preprocessed monitoring data are then stored for later use.

Operations which can be performed on a single orbit (or a single in-flight calibration dataset) are performed here. The input datasets are evaluated once they become available. All 1a, 1b, and in-flight calibration datasets shall be processed, so that the SPA data storage location contains a complete time series of the parameters relevant for long-term performance monitoring.

5.4.2.3 Variables

5.4.2.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Integration time index	i	-	t	-	
w	Spectral window index	i	-	t	-	

5.4.2.3.2 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N	Number of scans	i	-	t	-	
i_{Diff}	Pixel window for diffuser reflectivity monitoring	w[2]	pix	t	-	Start/end
j_{Diff}	Channel for pixel windows for diffuser reflectivity monitoring	enum	-	t	-	A window does not cross channel boundaries

5.4.2.3.3 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{HK}	Number of HK data words to be extracted (per Science Data Packet)	i	-	i	ini	
pos_{HK}	Positions (SDP word numbers) of HK data words to be extracted	$w[N_{\mathrm{HK}}]$	-	i	SPA ini	It is possible to use symbolic names for the HK fields in the ini dataset, and to perform the mapping to SDP word numbers internally.
$(\cos(2\chi_{ss}))_{\max}$	Upper limit for cosine of twice the polarisation angle for selected Stokes fractions	d	-	i	SPA ini	*0.026*
$P_{\mathrm{SS,min}}$	Lower limit for degree of polarisation for selected Stokes fractions	d	-	i	SPA ini	*0.1*
D_{1AU}	1 Astronomical unit	d	m	i	SPA ini	1.4959787×10^{11}

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$\lambda_{F,start}$	Start wavelength for fixed wavelength grid	d[B]	nm	i	SPA ini	Fixed grid will have *D* elements per channel.
$\lambda_{F,end}$	End wavelength for fixed wave-length grid	d[B]	nm	i	SPA ini	Fixed grid will have D elements per channel.
K_{PMD}	Co-adding factor for solar PMD readouts	i	-	i	SPA ini	*1*
lat_{E}	Minimum/maximum latitude for level 1b earthshine data selection.	d[2]	degree	i	SPA ini	
lon_{E}	Min/max longitude for level 1b earthshine data selection.	d[2]	degree	i	SPA ini	
lon_{SAA}	SAA longitude range (min/max)	d[2]	degree	i	SPA ini	*(–100, 0)*
lat_{SAA}	SAA latitude range (min/max)	d[2]	degree	i	SPA ini	*(–50, +10)*
N_{w}	Number of spectral windows for diffuser reflectivity monitoring	i	-	i	SPA ini	
λ_{Diff}	Spectral windows for diffuser reflectivity monitoring	d[N_{w},2]	nm	i	SPA ini	

5.4.2.3.4 Input from level 1a Product

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$D_{\mathrm{Sat\text{-}Sun}}$	Distance between satellite and sun	d	m	i	A4.1.1	**MDR-1a-Sun** GEO_SUNDISTANCE_SAT_SUN

5.4.2.3.5 Input from level 1b Product

All measurements in any of the calibration modes, except dark mode, are read completely. **MDR-1b-Calibration**, **MDR-1b-Sun**, **MDR-1a-Moon**

5.4.2.3.6 Input from in-flight calibration datasets

All available in-flight calibration data are read completely. In the case that the storage location for the in-flight calibration data and the SPA is the same, only Dark, SMR, and Etalon in-flight calibration data have to be read. **VIADR-1a-Dark**, **VIADR-1a-PPG**, **VIADR-1a-Spec**, **VIADR-1a-Etalon**, **VIADR-SMR.**

5.4.2.3.7 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
O	Electronic offset	d[B]	BU	o	A4.1.9	
L	Leakage current	d[B]	BU	o	A4.1.9	
λ_F	Fixed wavelength grid	d[D,B]	BU	o	A4.1.9	

5.4.2.4 Algorithm

A summary of the preprocessing steps being performed on the individual input data is given in the following table (Y = step is performed, N = step is not performed). Only selected housekeeping data, Stokes fractions, and spectra in earth mode will be extracted. The order of the algorithms below is also the sequence in which they have to be executed. Note that for the determination of the spectral reflectivity of the diffuser plate, measurements in SLS (direct) and SLS over diffuser mode have to be combined.

Algorithm step	Ref.	1a		1b							In-flight cal				
		HK	Stokes	Earth	Sun	WLS	SLS	SLS diff	LED	Moon	Dark	SMR	Etalon	PPG	Spectral
SPA Extraction and Pre-processing	**A4.1**	**selected data**			**all data**										
Extract Monitoring Data	A4.1.1	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Pre-Process Housekeeping Data per Scan	A4.1.2	Y	N	N	N	N	N	N	N	N	N	N	N	N	N
Average Valid Spectral Data per Observation Mode	A4.1.3	N	N	Y	N	Y	Y	Y	Y	Y	N	N	N	N	N
Interpolate Spectral Data to Fixed Wavelength Grid	A4.1.4	N	N	Y	N	Y	Y	Y	Y	Y	N	Y	Y	N	N
Normalise Solar and Earth Spectral Data to Solar Distance 1 AU	A4.1.5	N	N	Y	N	N	N	N	N	N	N	Y	N	N	N
Determine Stokes Fractions for Solar Measurements	A4.1.6	N	N	N	Y	N	N	N	N	N	N	N	N	N	N
Determine Spectral Reflectivity of Diffuser Plate	A4.1.7	N	N	N	N	N	Y		N	N	N	N	N	N	N
Pre-Process Dark Signal Measurements	A4.1.8	N	N	N	N	N	N	N	N	N	Y	N	N	N	N
Write Pre-processed Monitoring Data	A4.1.9	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y

5.4.2.5 EXTRACT MONITORING DATA (A4.1.1)

Input and data granule:

One level 1a or level 1b product or one or more in-flight calibration datasets.

Output:

Monitoring data for steps A4.1.2 to A4.1.9.

5.4.2.6 Algorithm:

Depending on the dataset(s) being available on input, extract the following data.

Level 1a product:

- Housekeeping data according to selection in initialisation dataset.
- Stokes fractions for special earth viewing geometries: Using the cosine of the double polarisation angle $\cos(2\chi_{SS})$ and the single-scattering degree of polarisation P_{SS}, extract the Stokes fractions q for those measurements where

$$\left|\cos(2\chi_{SS})\right| < (\cos(2\chi_{SS}))_{max} \text{ and } P_{SS} > P_{SS,min} .$$

The separation into scans shall be retained. For each parameter, the time $t_{\psi,0}$ corresponding to the first scanner position within a scan (i.e., the record start time given in the Measurement Data Record) shall be considered as time tag.

Level 1b product:

Extract earth measurements within the geographical region defined by lat_E and lon_E.

Extract measurements in any calibration mode except dark mode:

- Sun and Moon
- WLS
- SLS (direct)
- SLS via diffuser
- LED
- Moon

For all measurements in calibration mode, scans flagged to be within the South Atlantic Anomaly (**MDR_*** PCD_BASIC F_SAA) as defined by lat_{SAA} and lon_{SAA} shall be excluded. For measurement in WLS (SLS) mode, scans within the stabilisation time t_{stab}^{WLS} (t_{stab}^{SLS}) as determined from the lamp current, shall be excluded.

Measurements in dark mode do not have to be extracted because the dark in-flight calibration datasets already contain all the information relevant for long-term performance monitoring.

As for the level 1a product, the separation into scans shall be retained, and for each parameter, the time $t_{\psi,0}$ corresponding to the first scanner position within a scan (i.e., the record start time given in the Measurement Data Record) shall be considered as time tag.

In-flight calibration dataset:

- Dark: Extract all data. As data are separated into in-flight calibration datasets per channel and integration time, this means, several in-flight calibration datasets have to be read.
- SMR: Extract all data.
- Etalon: Extract all data.
- PPG: Extract all data.
- Spectral calibration parameters: Extract all data. The start time of the respective measurement, as specified in the in-flight calibration dataset, shall be considered as time tag.

Only dark signals, SMR, and Etalon data will be preprocessed below. PPG and spectral calibration parameters will be written to the SPA data storage location without modifications.

Note: In the case that the same storage location is used for in-flight calibration data and SPA data, this means PPG and spectral calibration data do not have to be extracted or written to the data storage location.

5.4.2.7 PRE-PROCESS HOUSEKEEPING DATA PER SCAN (A4.1.2)

Input and data granule:

One scan of selected housekeeping data from level 1a products..

Output:

Condensed housekeeping data.

5.4.2.8 Algorithm:

For each of the selected housekeeping data, convert housekeeping data from engineering units to physical units using Convert Housekeeping Data (AG.4).

For each of the housekeeping data in physical units, calculate per scan: mean, standard deviation, minimum and maximum values.

Derive on/off status flags per scan for SLS, WLS, and LED from their status bits in the HK data and their voltage and current values. Results shall be given separately for the available LED chains (1N, 2N, 1R, 2R), and WLS currents (360, 300, 400, 420 mA). A light source shall be considered “on” in a scan, if in at least one of the packets in the scan the respective status bit is indicating status “on”. For the SLS and WLS it is also required that their respective voltage is above a given threshold.

Derive open/closed status flags for the shutter per scan. The shutter shall be considered “open” in a scan, if in at least one of the packets in the scan the respective status bit is indicating status “open”

5.4.2.9 AVERAGE VALID SPECTRAL DATA PER OBSERVATION MODE (A4.1.3)

Input and data granule:

Selected spectral data from level 1a products.

Output:

Averaged spectrum for this observation mode.

5.4.2.10 Algorithm

Calculate the mean and standard deviation for each channel using Calculate Mean, Standard Deviation and Mean Error of Readouts (AX.1).

5.4.2.11 INTERPOLATE SPECTRAL DATA TO FIXED WAVELENGTH GRID (A4.1.4)

Input and data granule:

Spectral data S with associated wavelength grid λ. This is data coming from level 1b or SMR or Etalon in-flight calibration data.

Output:

Interpolated spectral data S on fixed wavelength grid λ_F.

5.4.2.12 Algorithm

Loop information: The calculations that follow are performed for all channels j.

Create the fixed wavelength grid. The number of points in the fixed wavelength grid is D_j, and the grid points are defined by the following:

$$\lambda_{F,ij} = \lambda_{F,start,j} + i \cdot \frac{\lambda_{F,end,j} - \lambda_{F,start,j}}{D_j - 1} \qquad (i = 0 \ldots D_j - 1)$$

Equation 237

Interpolate the spectral data S from its grid λ to the fixed grid λ_F using Spline Interpolation (AX.3), yielding interpolated signals $\hat{S}$. For fixed grid points not covered by the original grid λ, set the signal to a predefined value indicating no data are available.

End of loop.

Note: On fixed grid selection (i.e., choice of initialisation parameters): The wavelength range $\lambda_{F.start}$, $\lambda_{F,end}$ should be within the wavelength range covered by the respective channel, with some margin at the channel edges in order to account for expected in-orbit spectral drifts. In this way, interpolation should usually be possible to all fixed grid points.

5.4.2.13 NORMALISE SOLAR AND EARTH SPECTRAL DATA TO SOLAR DISTANCE 1 AU (A4.1.5)

Input and data granule:

Spectrally interpolated signals from SMR or selected earth data.

Output:

Signals normalised to a solar distance of 1 Astronomical Unit.

5.4.2.14 Algorithm

Normalise spectrally interpolated signals $\hat{S}$ from the sun and the selected data from the earth to a solar distance of 1 Astronomical Unit:

$$S_{1\text{AU},ij} = \left(\frac{D_{\text{Sat-Sun}}}{D_{1\text{AU}}}\right)^2 \cdot \hat{S}_{ij}$$

Equation 238

5.4.2.15 DETERMINE STOKES FRACTIONS FOR SOLAR MEASUREMENTS (A4.1.6)

Input and data granule:

Measurements in Sun mode (not averaged, not the SMR).

Output:

Stokes fractions for solar measurements.

5.4.2.16 Algorithm

The Stokes fractions for the solar measurements – which can be in any of the PMD transfer modes– are calculated as follows:

- PMD signals from solar observation mode are selected by the intensity in main channel 3 as in the calculation of the Solar Mean Reference Spectrum (see A2.20.2). This leaves N_{Sun} PMD readouts to be processed further. Any PMD transfer mode can be used.

Loop information: The following calculations are performed for all PMD bands (in the case that the transfer mode is band+raw or band+mixed), or for all PMD pixels (in the case that the transfer mode is raw).

- If $K_{PMD} > 1$, co-add K_{PMD} PMD readouts in time (N_{Sun} readouts in the case $K_{PMD} > N_{Sun}$).
- The Stokes fraction is calculated using Equation 176. In the case that the PMD transfer mode is "band", band integrated Müller matrix elements have to be used.

End of loop.

5.4.2.17 DETERMINE SPECTRAL REFLECTIVITY OF DIFFUSER PLATE (A4.1.7)

Input and data granule:

Averaged spectrum in SLS (direct) mode, averaged spectrum in SLS over diffuser mode.

Output:

Spectral reflectivity of diffuser plate for several spectral windows.

5.4.2.18 Algorithm

Using averaged main channel measurements in SLS over diffuser mode and measurements in SLS direct mode not more than one orbit apart, derive the spectral diffuser reflectivity as follows:

Loop information: The calculations are performed for all spectral windows *w*.

Using the dispersion relation for the main channels, find the pixel ranges $i_{\mathrm{Diff},1}$, $i_{\mathrm{Diff},2}$ and detector number j_{Diff} corresponding to window boundaries $\lambda_{\mathrm{Diff},w,1}$, $\lambda_{\mathrm{Diff},w,2}$. (The wavelengths corresponding to $i_{\mathrm{Diff},1}$, $i_{\mathrm{Diff},2}$ shall be within the range $\lambda_{\mathrm{Diff},w,1}$, $\lambda_{\mathrm{Diff},w,2}$, and the wavelengths corresponding to $i_{\mathrm{Diff},1} - 1$, $i_{\mathrm{Diff},2} + 1$ outside this range.)

Sum each of the two spectra in the detector pixel domain into spectral window *w* as follows:

$$S_w^{\mathrm{direct}} = \sum_{i=i_{\mathrm{Diff},1}}^{i_{\mathrm{Diff},2}} S_{ij_{\mathrm{Diff}}}^{\mathrm{direct}}$$ *Equation 239*

$$S_w^{\mathrm{Diff}} = \sum_{i=i_{\mathrm{Diff},1}}^{i_{\mathrm{Diff},2}} S_{ij_{\mathrm{Diff}}}^{\mathrm{Diff}}.$$ *Equation 240*

Divide the summed signal from the measurement over diffuser by the summed signal from the direct measurement:

$$R_w = \frac{S_w^{\mathrm{Diff}}}{S_w^{\mathrm{direct}}}$$ *Equation 241*

End of loop.

Note: On spectral window selection (i.e., choice of initialisation parameters): A spectral window shall not cross channel boundaries. Windows shall be wide enough to give sufficient signal to noise ratios (this is particularly important in the UV). Window boundaries shall not coincide with spectral lines. This ensures that results are not sensitive to spectral drifts, and measurements from the two modes (SLS and SLS over diffuser) can be combined independent of their respective pre-disperser prism temperatures.

5.4.2.19 PRE-PROCESS DARK SIGNAL MEASUREMENTS (A4.1.8)

Input:

Dark signals from in-flight calibration datasets, at several integration times, not more than one orbit apart.

Output:

Electronic offset and leakage current.

Data Granule:

Dark in-flight calibration datasets, not more than one orbit apart.

5.4.2.20 Algorithm

Loop information: The following is performed for all bands *j* and all detector pixels *i* within a band.

Using dark signals measured not more than one orbit apart at the same detector temperature, but at different integration times IT_k, separate into electronic offset (in BU) and leakage current (inBU/s) as follows:

Perform a least-squares fit of a linear function of the integration time IT_k to the dark signal S_{ijk}, where the electronic offset O_{ij} and the leakage current L_{ij} are the fit parameters:

$$\sum_k (L_{ij} IT_{jk} + O_{ij} - S_{ijk})^2 \stackrel{!}{=} \min \quad \text{Equation 242}$$

End of loop.

5.4.2.21 Write pre-processed monitoring data (A4.1.9)

Input and data granule:

Monitoring information from steps A4.1.1 to A4.1.8.

Output:

N/A

5.4.2.22 Algorithm

The monitoring information is stored in the SPA data storage location.

5.4.3 SPA ANALYSIS (A4.2)

Input:

Monitoring information from SPA data storage location.

Output:

Condensed monitoring information and degradation factors.

Uses Generic Sub-Functions:

Monitoring information from SPA data storage location.

Uses Auxiliary Sub-Functions:

None.

Data Granule

Subset of monitoring information for a specified timeframe.

5.4.3.1 Objectives

To retrieve monitoring information from the SPA data storage location and to perform analysis.

5.4.3.2 Description

This module provides the tools needed for the study of the long-term instrument performance monitoring. Monitoring information is extracted for a given timeframe which may extend from a few orbits to several years of data. The monitoring information is then evaluated and condensed by statistical analysis. Analysis on the housekeeping data is performed in order to diagnose the instrument health from an engineering point of view, covering thermal, electrical, and mechanical aspects, and maintaining a usage statistics for life-limited items. Spectral data are analysed in order to monitor the optical properties of the instrument, and ultimately to derive correction factors to compensate for instrument degradation in the level 0 to 1 processing.

5.4.3.3 Variables

5.4.3.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
m	Polynomial coefficient index	i	-	t	-	0…M
n	Index of element within time series					0…N–1

5.4.3.3.2 Local Variable

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N	Number of elements in time series	i	-	t	-	
t	Time	d[N]	days	t	-	
t_0	SLS ignition start time	d	days	t		
t_1	SLS ignition end time	d	days	t	-	
p	Parameter in time series	d[N]	(various)	t	-	

5.4.3.3.3 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
I^{SLS}_{low}	Lowest nominal SLS lamp current	d	A	i/o	SPA ini	9.5×10^{-3}
U^{SLS}_{on}	Minimum SLS voltage for the SLS to be considered “on”	d	V	i/o	SPA ini	20

5.4.3.3.4 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
F	Indicator for function used in the fit (polynomial, sine, exponential, …)	enum	-	o	A4.2.17	
c	Fit coefficients	d[10]	(various)	o	A4.2.17	Typically, only the first 2–4 elements will be used.
M	Order of polynomial fitted to time series	i	-	o	A4.2.17	Only used if polynomial function has been fitted.

5.4.3.4 Algorithm

Relevant monitoring information for a user-defined timeframe is extracted from the SPA data storage location and the resulting time series is analysed statistically as described below. The time interval for the analysis is the user-defined time frame, unless indicated otherwise. For the spectral data, both main channels and PMD channels have to be considered, unless indicated otherwise. This section is organised into groups of parameters to be monitored, called monitoring topics below, with the exception of the first subsection (A4.2.1) which summarises the statistical algorithms used throughout the SPA analysis.

5.4.3.4.1 PERFORM STATISTICAL ANALYSIS ON TIME SERIES (A4.2.1)

The elements for the statistical analysis which have to be available for the SPA analysis are described here.

Frequently, the parameter to be analysed is not a scalar (e.g., temperature), but a one-dimensional or two-dimensional array (e.g., signal values, leakage currents, pixel-to-pixel gain values), there is a time series for each element of the array. The SPA analysis tool shall be able to handle these cases by performing the analysis described below per element of the input array, giving an array of the same shape (number of elements and dimensions) on output.

Note: This concept is called “elemental function reference” in Fortran-90.

5.4.3.4.2 Basic Statistics

Given a series of parameters p_n (anything except flags and counters from the storage location, e.g., temperatures, voltages, signal values, leakage currents) with associated time stamps t_n ($n = 0,\dots, N-1$), the SPA analysis tool shall be able to calculate these values:

- mean value $\bar{p} = \frac{1}{N}\sum_n p_n$
- standard deviation stddev(p) = $\sqrt{\frac{1}{N-1}\sum_n (p_n - \bar{p})^2}$
- minimum value (p)
- maximum value (p)

5.4.3.4.3 Modelling the time series

Least-squares fitting routines shall be provided for the analysis of the time series, as a minimum:

- Linear fit of a polynomial function of order M with $M + 1$ coefficients c_m (this includes as a special case $M = 1$, the determination of a linear trend):

$$\sum_{n=0}^{N-1}\left(\sum_{m=0}^{M} c_m (t_n - t_0)^m - p_n\right)^2 \stackrel{!}{=} \min$$

Equation 243

- Non-linear fit of periodic function (amplitude c_0, phase c_1):

$$\sum_{n=0}^{N-1}\left(c_0\sin\left(\frac{t_n-t_0-c_1}{2\pi T}\right)-p_n\right)^2 \stackrel{!}{=} \min$$

Equation 244

The periodicity T shall not be a fit parameter but selectable by the user–one orbit, one year (see below).

- Non-linear fit of exponential function (value at $t = t_0$: c_0, 1/e decay time: c_1):

$$\sum_{n=0}^{N-1}\left(c_0 e^{-(t_n-t_0)/c_1}-p_n\right)^2 \stackrel{!}{=} \min$$

Equation 245

For the linear fits, functions similar to the singular value decomposition and back substitution functions from [RD 9] should be employed. For the non-linear fits, functions similar to the Levenberg-Marquardt routines from [RD 9] should be employed.

When the particular function to be fitted is not indicated in the sections that follow, the understanding is that the operator of the SPA analysis tool chooses and optimises this function according to the observed temporal behaviour of a given parameter. Therefore, the function to be fitted shall not be hard-coded per parameter, but selectable by the operator.

5.4.3.4.4 Read Pre-Processed Monitoring Data (A4.2.2)

On start-up, the operator shall be presented with a list of the available monitoring topics (A4.2.3 to A4.2.16), from which he/she has to select one. The parameters relevant for this topic are then read from the SPA data storage location.

5.4.3.4.5 Monitor housekeeping data (A4.2.3 to A4.2.6)

5.4.3.4.5.1 DERIVE USAGE STATISTICS FOR LIFE-LIMITED ITEMS AND MODE STATISTICS (A4.2.3)

For SLS, WLS, and LED, calculate from their on/off status flags the total duration they were switched on and the number of times they were switched on. The total switch-on duration is the number of scans with the respective status flag set “on” multiplied by the scan duration (6s). The number of times they were switched on is the number of transitions from “off” to “on” status flag. Results shall be given separately for the available LED chains (1N, 2N, 1R, 2R), and WLS currents (360 mA, 380 mA, 400 mA, 420 mA).

For the scanner, calculate the total number of scans in any of the four earth scanning modes. Forth shutter, calculate the total number of actuations, both in nominal mode and in emergency mode, and the total duration when the shutter was open.

Using the instrument mode from the level 1a product, calculate the total number of scans per mode, the total duration per mode, and its percentage of the total measurement time (sum of duration for all modes).

5.4.3.4.6 Monitor Thermal Performance (A4.2.4)

Analyse the time series of selected temperatures other than the detector temperatures, e.g., predisperser prism, radiator, and optical bench temperatures. Determine the amplitudes and phases of orbital and seasonal variations for these temperatures using equation (244) with T set to the duration of one orbit or to one year respectively.

Analyse the time series of detector array temperatures and the Peltier loop output for the measurements where the respective cooler is switched on.

5.4.3.4.7 Monitor Electrical Performance (A4.2.5)

Analyse the time series of SLS and WLS voltages and currents, per switch-on period and as a long-term time series. Derive SLS ignition delay and ignition voltage from SLS voltage and current values and analyse their time series. Analyse time series of Housekeeping Data Module offset and gain values.

Note: On ignition parameters, The SLS is a gas discharge lamp. The gas mixture (Ne/Ar) needs to be ignited first at a high voltage before the current begins to flow. When the SLS is switched on, the voltage is controlled such that it increases linearly in time. If t_0 is the UTC timestamp (in days) of the first packet where the SLS voltage exceeds U_{on}^{SLS}, and t_1 (> t_0) is the UTC time stamp (in days) of the first packet where the SLS current exceeds I_{low}^{SLS}, the *ignition delay* (in seconds) is defined by ($t_1 - t_0$) times the number of seconds per day. The *ignition voltage* is the maximum SLS voltage reached between t_0 and t_1 (the packets at t_0 and t_1 being included in the comparison).

5.4.3.4.7.1 MONITOR SCANNER PERFORMANCE (A4.2.6)

For static modes, analyse time series of scanner position with respect to the set value. For earth scanning mode, compare the scanner positions across the scan with the expected values, calculate the deviations, and analyse the resulting time series.

5.4.3.4.8 Monitor spectral data (Main channels and PMD channels) (A4.2.7 to A4.2.14)

5.4.3.4.8.1 MONITOR DARK SIGNALS (A4.2.7)

Select dark signal data (electronic offsets, leakage current and dark signal noise) within a user-specified detector temperature range and – for the dark signal noise – a given integration time.

Note: In the preprocessing step A4.1.8, dark signal measurements from different integration times have been reduced to offset [BU] and leakage [BU/s]. So for offset and leakage, integration time is no longer a parameter.

Analyse time series of electronic offsets, leakage current and dark signal noise (all per detector pixel). It shall be possible to analyse both noise per detector pixel (i,j) and the noise averaged per band (j).

5.4.3.4.8.2 MONITOR SIGNALS FROM INTERNAL LIGHT SOURCES (A4.2.8)

Analyse time series of signals of internal light sources (SLS, WLS, LED). Within a time series, the integration time, time after lamp stabilisation, and (for the WLS) lamp current have to be identical.

5.4.3.4.8.3 MONITOR SPECTRAL STABILITY (A4.2.9)

Using the spectral calibration polynomials, calculate from equation (376) wavelengths for selected detector pixels per channel and analyse their time series.

5.4.3.4.8.4 MONITOR ETALON AND ETALON RESIDUALS (A4.2.10)

Analyse time series of Etalon spectra and Etalon residuals.

5.4.3.4.8.5 MONITOR PIXEL-TO-PIXEL GAIN (A4.2.11)

Analyse time series of the pixel-to-pixel gain (per detector pixel).

5.4.3.4.8.6 MONITOR DIFFUSER REFLECTIVITY (A4.2.12)

Analyse time series of the diffuser reflectivity (per spectral window).

5.4.3.4.8.7 MONITOR INSTRUMENT THROUGHPUT USING SOLAR MEASUREMENTS (A4.2.13)

Calculate ratios of solar spectra with a reference solar spectrum. Separate broadband and narrow-band effects in the ratios by subtracting a low-order polynomial in the spectral domain:

$$\sum_{i=0}^{D-1}\left(\sum_{m=0}^{M} c_m(\lambda_n-\lambda_0)^m - S_{ij}\right)^2 \stackrel{!}{=} \min$$

Equation 246

Analyse time series of both components at selected wavelengths. Check for periodicities (e.g., annual).

5.4.3.4.8.8 MONITOR INSTRUMENT THROUGHPUT USING EARTHSHINE MEASUREMENTS (A4.2.14)

Select earthshine spectra for a given scene specified by swath width and ranges for latitude, longitude, and solar zenith angle (topocentric CS). Calculate ratios of selected earthshine spectra for a given scene and viewing angle with a reference earthshine spectrum for the same scene (at a different time) and viewing angle. Do the same for earthshine albedos (earth/sun ratios). Analyse time series (per viewing angle).

5.4.3.4.9 Monitor polarisation data (A4.2.15 to A4.2.16)

5.4.3.4.9.1 MONITOR STOKES FRACTIONS OF SOLAR MEASUREMENTS (A4.2.15)

Analyse time series of Stokes fractions of solar measurements (per PMD pixel or band). As solar radiation (when observed from space) is known to be unpolarised, the Stokes fractions should be zero within the measurement error for all PMD pixels (bands).

5.4.3.4.9.2 MONITOR POLARISATION FOR SPECIAL EARTH VIEWING GEOMETRIES (A4.2.16)

Analyse time series of Stokes fractions extracted for the special earth viewing geometries (see above). For these geometries, the Stokes fractions should be close to zero within the measurement error for all PMD bands.

5.4.3.4.9.3 WRITE CONDENSED MONITORING INFORMATION AND DEGRADATION CORRECTION FACTORS (A4.2.17)

Condensed monitoring information is to be written in ASCII text datasets or stored in the SPA data storage location (selection by the operator). This comprises the start and end of the operator-selected timeframe for the analysis, and for each parameter analysed the results from the statistical analysis (A4.2.1), i.e., mean/min/max values, standard deviation, indicator for function fitted(enumerated variable), and fit coefficients.

5.5 PRODUCT QUALITY EVALUATION (A5)

5.5.1 PROCESSING OVERVIEW

The Product Quality Evaluation (PQE) functionality shall provide information about the quality of the generated level 1 data products. A number of checks are performed during Level 0 to 1a Processing (A2) and Level 1a to 1b Processing (A3) and the results are stored in Product Confidence Data records (PCDs) in the Level 1a and Level 1b data products. PCDs are provided both at the product and scan level. PCDs containing information about the quality of applied calibration parameters are also included. A pre-processing functionality extracts the PCDs directly after processing of the level 1a and 1b data products and updates the PQE storage location with the extracted data. A second functionality further condenses the extracted data to provide daily, weekly, monthly and yearly Product Quality Summaries and “Quick-Look” information. The highest level of detail, on measurement pixel level, is not covered by automatic PQE functionality.

Figure 17 gives a high-level description of data flow which is required for the PQE functionality.

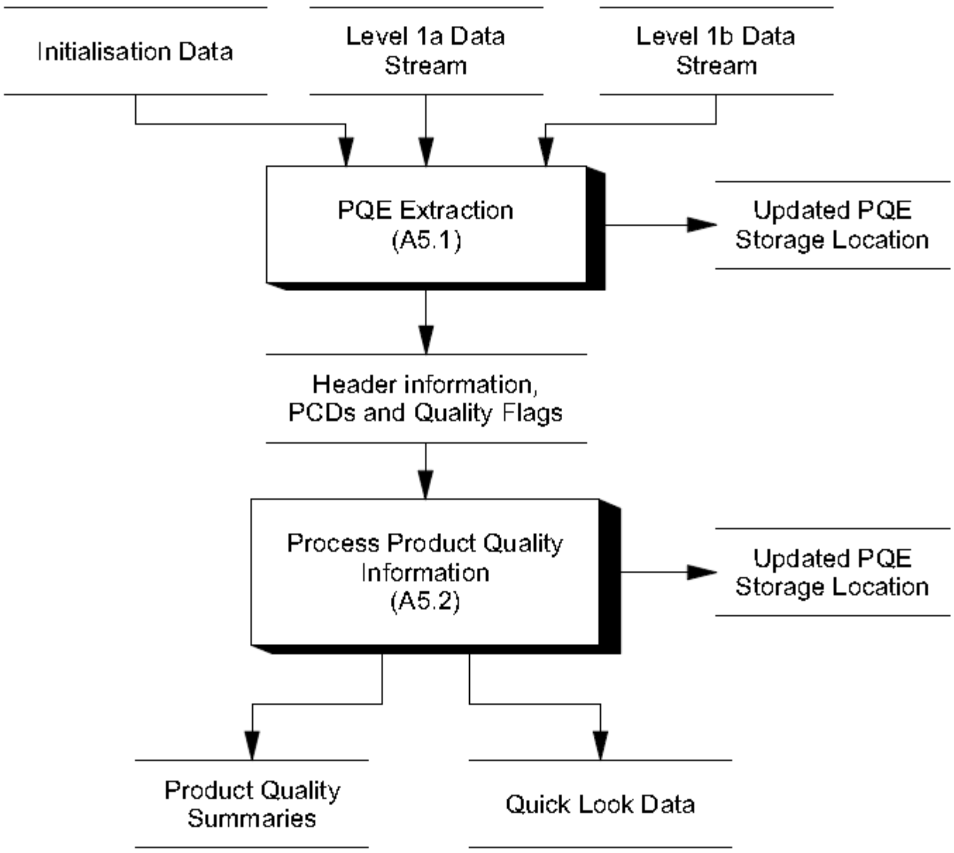

Figure 17: A5 Functional Decomposition: PQE functionality.

5.5.2 PQE EXTRACTION (A5.1)

Input:

Initialisation data. Level 1a and level 1b products.

Output:

Product header information, PCDs both on a global and scan basis and PCDs providing information about the quality of applied calibration parameters. A selected subset of Earthshine measurements for the calculation of "Quick-Look" information and initialisation parameters. Updated PQE storage location.

Uses Generic Sub-Functions:

None.

Uses Auxiliary Sub-Functions:

None.

Data Granule

One Product.

5.5.2.1 Objectives

To extract header information, all PCD records, and a selected sub-set of Earthshine measurements from the level 1a and 1b data products as specified in equation [AD4] and equation [AD5],to be used in the generation of Product Quality Summary and "Quick-Look" information. The extracted data are written to the PQE storage location. Initialisation parameters are also read frogman initialisation dataset.

5.5.2.2 Description

A number of checks are performed during Level 0 to 1a Processing (A2) and Level 1a to 1b Processing (A3) and the results are stored in Product Confidence Data records in the level 1a and level 1b data products. PCDs are provided both at the product and scan level. PCDs containing information about the quality of applied calibration parameters are also included. This pre-processing functionality extracts the PCDs and other selected parameters directly after processing of the level 1a and 1b data products, writes the information to the PQE storage location and makes it available for the generation of Product Quality Summaries and "Quick-Look" information as described in Section 5.5.3.

The product header information and PCDs required from the level 1a and level 1b data products are listed in Section 5.5.2.3. Data are extracted on four levels as indicated: product header information and global PCDs, PCDs containing information about the in-flight calibration data stored in Variable Internal Auxiliary Data Records, PCDs applicable to the scan level, and a selected sub-set of Earthshine measurements, from the level 1a and 1b data products. Variable tables below are presented by extraction level.

The PQE storage location will store Product Quality data for the lifetime of the mission and make it available for visualisation and analysis.

5.5.2.3 Variables (Extract Product Header Information and Global PCDs (A5.1.2)

5.5.2.3.1 Input from Level 1a and Level 1b Product

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
Prod_ID	Product Identifier	i	-	i/o	lv1a and lv1b / PQE store	**MPHR** PRODUCT_NAME
Start_Orbit	Start Orbit number of product			i/o	lv1a and lv1b / PQE store	**MPHR** ORBIT_START
End_Orbit	End Orbit number of product			i/o	1v1a and lv1b / PQE store	**MPHR** ORBIT_END
Start_time	Start UTC date/time of product	d	fractional days	i/o	1v1a and lv1b / PQE store	**MPHR** SENSING_START_DUMP
End_time	End UTC date/time of product	d	fractional days	i/o	1v1a and lv1b / PQE store	**MPHR** SENSING_END_DUMP

5.5.2.3.2 Global PCD Records from Level 1a and 1b Product

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
N_{scan}	Number of scans in the product	w	-		A3.0.4/A3.17.3	**SPHR** N_SCANS
N_{val_dp}	Number of valid scans with missing data packets	w	- i/o	i/o	A3.0.4/A3.17.3	**SPHR** N_VALID_WITH_MISS_DP
N_{miss_dp}	Number of missing data packets invalid scans	w	-		A3.0.4/A3.17.3	**SPHR** N_MISS_DP
N_{miss_scan}	Number of missing scans	w	- i/o	i/o	A3.0.4/A3.17.3	**SPHR** N_MISSING_SCANS
N_{nn_dt}	Number of scans with non-nominal detector temperature	w[B]	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_NN_DETECTOR_TEMP

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{nn_pdp}	Number of scans with non-nominal pre-disperser prism temperature	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_NN_PDP_TEMP
N_{nn_rad}	Number of scans with non-nominal radiator temperature	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_NN_RAD_TEMP
N_{nn_WLSU}	Number of scans with non-nominal WLS lamp voltage	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_NN_WLS_U
N_{nn_WLSI}	Number of scans with non-nominal WLS lamp current	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_NN_WLS_I
N_{nn_SLSU}	Number of scans with non-nominal SLS lamp voltage	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_NN_SLS_U
N_{nn_SLSI}	Number of scans with non-nominal SLS lamp current	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_NN_WLS_I
N_{inv_UTC}	Number of scans with invalid UTC	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_INV_UTC
N_{Nad_scan}	Number of scans in *Nadir_scan* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_NADIR_SCAN
N_{Nth_scan}	Number of scans in *Nth_pole_scan* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_NTH_POLE_SCAN
N_{Sth_scan}	Number of scans in *Sth_pole_scan* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_STH_POLE_SCAN
N_{Oth_scan}	Number of scans in *Other_scan* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_OTHER_SCAN
N_{Nad_static}	Number of scans in *Nadir_static* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_NADIR_STATIC
N_{Oth_static}	Number of scans in *Other_static* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_OTHER_STATIC

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
N_{Dark}	Number of scans in Dark observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_DARK
N_{LED}	Number of scans in *LED* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_LED
N_{WLS}	Number of scans in *WLS* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_WLS
N_{SLS}	Number of scans in *SLS* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_SLS
N_{SLS_diff}	Number of scans in *SLS* over diffuser observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_SLS_DIFF
N_{Sun}	Number of scans in *Sun* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_SUN
N_{Moon}	Number of scans in *Moon* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_MOON
N_{Idle}	Number of scans in *Idle* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_IDLE
N_{Test}	Number of scans in *Test* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_TEST
N_{Dump}	Number of scans in *Dump* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_DUMP
$N_{Invalid}$	Number of scans assigned *Invalid* observation mode	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_INVALID
N_{sat}	Number of scans with saturated pixels. For PMDs the nominal range (blocks CD) are separated from the remainder (blocks DE)	w[B]	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_SATURATED
N_{hot}	Number of scans with hot pixels	w[B]	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_HOT

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{min}	Number of scans where the mean uncalibrated signal is below a specified threshold per band	w[B]	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_MIN_INTENSITY
N_{SAA}	Number of scans in the SAA	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_SAA
$N_{sunglint}$	Number of scans with sunglint danger	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_SUNGLINT
$N_{rainbow}$	Number of scans with rainbow danger	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_RAINBOW
$N_{mode,geo}$	Number of scans with possible mismatch between observation mode and geolocation	w	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_MODE_GEOLOCATION
$N_{\mathrm{MissStokes}}$	Number of scans with missing Stokes fractions	w[N_{PMD}]	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_MISS_STOKES
$N_{\mathrm{BadStokes}}$	Number of scans with bad Stokes fractions	w[N_{PMD}]	-	i/o	lv1a and lv1b / PQE store	**SPHR** N_BAD_STOKES
N_{cloud}	Number of scans with fractional cloud above a specified threshold	w	-	i/o	lv1a and lv1b/PQE store	**SPHR** N_CLOUD

5.5.2.3.3 Extract PCDs from Variable in-flight Auxiliary Data Records (A5.1.3): PCD Records per VIADR from Level 1a and 1b Product

Input from in-flight calibration dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
DS_{start}	Start UTC date/time of valid Dark calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** START_UTC_DARK
DS_{end}	End UTC date/time of valid Dark calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** END_UTC_DARK
DS_{IT}	Integration time for which dark signal correction is valid	d[B]	s	i/o	lv1a and lv1b/PQE store	**VIADR-1a- Dark** INTEGRATION_TIME
DS_{dt}	Mean detector temperature for which dark signal correction is valid	d[B]	K	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** FPA_TEMP
$DS_{transfer}$	*pmd_transfer* mode for which dark signal correction is valid	enum	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** PMD_TRANSFER
$DS_{readout}$	*pmd_readout* mode for which dark signal correction is valid	enum	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** PMD_READOUT
$\overline{DS}$	Dark signal correction averaged per band.	d[B]	BU	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** PCD_DARK AV_DARK
$\overline{\sigma_D}$	Dark signal correction readout noise averaged per band.	d[B]	BU	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** PCD_DARKAV_DARK_NOISE
$F_{\overline{DS}}$	Flag indicating whether dark signal correction averaged per band exceeds specified threshold	bool[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** PCD_DARK F_AV_DARK 1 = exceeds 0 = does not
$F_{\overline{\sigma_D}}$	Flag indicating whether dark signal correction readout noise averaged per band exceeds specified threshold	bool[B]	-	i/o	lv1a and lv1b/PQE store	**IADR-1a-Dark** PCD_DARK F_AV_DARK_NOISE 1 = exceeds 0 = does not

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
F_D^{miss}	Flag indicating that missing mean *Dark* calibration mode measurements have been filled by interpolation or that one complete band is missing	enum[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Dark** PCD_DARK F_DARK_MISS
LED_{start}	Start UTC date/time of valid *LED* (or *WLS* if *PPG_back* = *WLS*) calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** START_UTC_PPG
LED_{end}	End UTC date/time of valid *LED* (or *WLS* if *PPG_back* = *WLS*) calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** END_UTC_PPG
PPG_back	Switch for selection of backup source (WLS) in event of LED failure	enum	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** PCD_PPGPPG_BACK
$\overline{PPG}$	Mean PPG correction per channel	d[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** PCD_PPGAV_PPG
σ_{PPG}	Standard deviation of PPG per channel	d[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** PCD_PPGSTDDEV_PPG
$F_{\overline{PPG}}$	Flag indicating whether PPG averaged per channel exceeds specified threshold	bool[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** PCD_PPGF_AV_PPG 1 = exceeds 0 = does not exceed
$F_{\sigma PPG}$	Flag indicating whether standard deviation of PPG per channel exceeds specified threshold	bool[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** PCD_PPGF_STDDEV_PPG 1 = exceeds 0 = does not exceed
F_{PPG}^{miss}	Flag indicating that missing mean *LED* calibration mode measurements have been filled by interpolation or that one complete channel is missing	enum[B]	-	i/o	lv1a and lv1b/PQE store	**IADR-1a-PPG** PCD_PPGF_PPG_MISS
F_{PPG}^{LED}	LED status flag	b	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-PPG** PCD_PPGF_PPG_LED See [AD 9]

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
SLS_{start}	Start UTC date/time of valid *SLS* calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** START_UTC_SLS
SLS_{end}	End UTC date/time of valid *SLS* calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** END_UTC_SLS
SLS_{pdp}	Mean pre-disperser prism temperature for which spectral calibration is valid	d[B]	K	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PDP_TEMP
N_{lines}	Number of lines accepted for use in spectral calibration per channel.	w[B_{FPA}]		i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECN_LINES
δ_{max}	Maximum deviation between fit-ted and true line position per channel	d[B_{FPA}]	nm	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECMAX_LINE_DEV
$\bar{\delta}$	Average deviation between fitted and true line position per channel	d[B_{FPA}]	nm	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECAV_LINE_DEV
δ	Deviation between fitted line position and true line positions.	d[N_{lines}, B_{FPA}]	nm	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECLINE_DEV
F_{lines}	Flag indicating whether number of lamp lines accepted for use in spectral calibration is below order of wavelength calibration polynomial *M* per channel.	bool[B_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECF_N_LINES 1 = number of lines too low 0 = number of lines sufficient
$F_{\delta_{max}}$	Flag indicating whether maximum deviation between fitted line positions and true line positions exceeds specified threshold.	bool[BFPA]		i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECF_MAX_LINE_DEV 1 = exceeds 0 = does not
F_{SLS}^{miss}	Flag indicating that no spectral calibration was generated due to missing mean SLS mode measurements per channel	bool[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECF_SPEC_MISS 1= no spectral calibration for given channel 0 = not missing

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{iter}	Number of iterations required for PMD spectral calibration per channel.	w[B_{PMD}]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECN_ITERATION
F_{noconv}	Flag indicating that PMD spectral calibration has not converged, per channel	bool[BPMD]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECF_NO_CONVERGENCE 1 = not converged 0 = converged
F_{gof}	Flag indicating whether quality of fit for PMD spectral calibration is above specified threshold	bool[BPMD]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Spec** PCD_SPECF_GOF 1 = goodness of fit too low 0 = goodness of fit acceptable
WLS_{start}	Start UTC date/time of valid WLS (or *Sun* if *Eta_back* = *Sun*) calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**IADR-1a-Etalon** START_UTC_WLS
WLSend	End UTC date/time of valid *WLS* (or *Sun* if *Eta_Back* = *Sun*) calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** END_UTC_WLS
Eta_algo	Etalon correction algorithm selection	i	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONETALON_BACK
Eta_back	Switch for selection of backup source (SMR) in event of WLS failure	enum	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONETALON_ALGO
$\overline{RES}$	Mean residual etalon per channel	d[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONAV_ETALON
σ_{RES}	Standard deviation of residual etalon per channel	d[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONSTDDEV_ETALON
$\overline{cppg}$	Mean residual structure at a pixel level	d[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONAV_RESIDUAL
σ_{cppg}	Standard deviation of residual structure at a pixel level	d[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONSTDDEV_RESIDUAL

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
$F_{\overline{RES}}$	Flag indicating whether mean residual etalon exceeds specified threshold per channel	bool[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONF_AV_ETALON 1 = exceeds 0 = does not
$F_{\sigma RES}$	Flag indicating whether standard deviation of residual etalon exceeds specified threshold per channel	bool[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONF_STDDEV_ETALON 1 = exceeds 0 = does not
$F_{\overline{PPS}}$	Flag indicating whether mean residual pixel level structure exceeds specified threshold per channel	bool[B]		i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONF_AV_RESIDUA L1 = exceeds 0 = does not
$F_{\sigma PPS}$	Flag indicating whether standard deviation in residual pixel level structure exceeds specified threshold per channel			i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONF_STDDEV_RESIDUAL 1 = exceeds 0 = does not
F^{miss}_{Eta}	Flag indicating that missing mean *WLS* calibration mode measurements have been filled by interpolation or that one complete channel is missing	enum[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-1a-Etalon** PCD_ETALONF_ETALON_MISS
Sun_{start}	Start UTC date/time of valid *Sun* calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-SMR** START_UTC_SUN
Sun_{end}	End UTC date/time of valid *Sun* calibration mode measurements	d	fractional days	i/o	lv1a and lv1b/PQE store	**VIADR-SMR** END_UTC_SUN
Sun_{trans}	PMD transfer mode associated with SMR	enum	-	i/o	lv1a and lv1b/PQE store	**VIADR-SMR** PMD_TRANSFER one enumerated value per scan
Sun_{read}	PMD readout mode associated with SMR	enum	-	i/o	lv1a and lv1b/PQE store	**VIADR-SMR** PMD_READOUT one enumerated value per scan
N_{sun}	Number of detector readouts in *Sun* observation mode which pass the intensity check test.	w	-	i/o	lv1a and lv1b/PQE store	**VIADR-SMR** PCD_SMRN_INTENSITY

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
F_{Nsun}	Flag indicating that number of detector readouts in *Sun* observation mode passing the intensity check test is too low.	bool	-	i/o	lv1a and lv1b/PQE store	**VIADR-SMR** PCD_SMRF_N_INTENSITY 1 = number of spectra too low 0 = number of spectra sufficient
F^{miss}_{Sun}	Flag indicating that no SMR was generated due to missing mean Sun mode measurements per channel	bool[B]	-	i/o	lv1a and lv1b/PQE store	**VIADR-SMR** PCD_SMRF_SMR_MISS 1 = no SMR for given channel 0 = not missing

5.5.2.3.4 EXTRACT PCDS PER SCAN AND READOUT (A5.1.4): PCD Records per Scan from Level 1a and 1b Products

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
Scan_Lon	Geocentric longitude for complete scan, ground, points ABCDF (earth-fixed CS)	d[5]	degrees	i	lv1a and lv1b/PQE store	**MDR-1b-Earthshine** GEO_EARTHSCAN_CORNER & SCAN_CENTRE
Scan_Lat	Geodetic latitude for complete scan, ground, points ABCDF (earth-fixed CS)	d[5]	degrees	i	lv1a and lv1b/PQE store	**MDR-1b-Earthshine** GEO_EARTH SCAN_CORNER& SCAN_CENTRE
Mode	Observation mode	enum	-	i/o	lv1a and lv1b/PQE store	**MDR-1*-** OBSERVATION_MODE
pmd_transfer	PMD transfer mode	enum	-	i/o	lv1a and lv1b/PQE store	**MDR-1*-** PMD_TRANSFER
pmd_readout	PMD readout mode	enum	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PMD_READOUT
F_{nn_dt}	Flag indicating non-nominal detector temperature	bool[B,R_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASIC F_NN_DT 1 = non-nominal 0 = nominal

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
F_{nn_pdp}	Flag indicating non-nominal predisperser prism temperature in scan	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_NN_PDP 1 = non-nominal 0 = nominal
F_{nn_rad}	Flag indicating non-nominal radiator temperature in scan	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_NN_RAD 1 = non-nominal 0 = nominal
F_{nn_WLSU}	Flag indicating non-nominal WLS voltage in scan	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_NN_WLS_U 1 = non-nominal 0 = nominal
F_{nn_WLSI}	Flag indicating non-nominal WLS current in scan	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_NN_WLS_I 1 = non-nominal 0 = nominal
F_{nn_SLSU}	Flag indicating non-nominal SLS voltage in scan	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_NN_SLS_U 1 = non-nominal 0 = nominal
F_{nn_SLSI}	Flag indicating non-nominal SLS current in scan	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_NN_SLS_I 1 = non-nominal 0 = nominal
F_{inv_UTC}	Flag for invalid UTC	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_INV_UTC 1 = invalid 0 = valid
F_{miss}	Flag for missing data packets	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASIC F_MISS 1 = missing 0 = none missing
F_{sat}	Flag indicating saturated pixels per band.	bool[B,R_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_SAT 1 = saturation 0 = no saturation
F_{hot}	Flag indicating hot pixels per band.	bool[B,R_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_HOT 1 = hot 0 = not hot

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
F_{min}	Flag indicating that the minimum mean uncalibrated signal is below a specified threshold per band	bool[B, R_{FPA}]	-	i/o	lv1b / PQE store	**MDR-1*** PCD_BASIC F_MIN 1 = below threshold 0 = above threshold
$\bar{S}$	Mean raw signal per band	w[B]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASIC MEAN_UC
F_{SAA}	Flag indicating scan is in SAA	bit-string [32]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_SAA 1 = SAA 0 = not SAA
$F_{sunglint\_risk}$	Flag indicating risk of sunglint	enum[R_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASIC F_SUNGLINT_RISK
$F_{sunglint\_high\_risk}$	Flag indicating high risk of sunglint	enum[R_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_SUNGLINT_ HIGH_RISK
$F_{rainbow}$	Flag indicating danger of rainbow	bool[R_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_RAINBOW 1 = risk 0 = no risk
$F_{mode,geo}$	Flag indicating possible mismatch between observation mode and geolocation	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*** PCD_BASICF_MODE_GEOLOCATION 1 = mismatch 0 = match
$F_{MissStokes}$	Flag indicating missing Stokes fractions in scan (per PMD band).	bool[N_{PMD}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*-Earthshine** PCD_EARTHF_MISS_STOKES 1 = some missing 0 = all present
$F_{BadStokes}$	Flag indicating bad Stokes fractions in scan. Bad Stokes fractions are those which have been calculated but seem suspicious compared to the expectations	bool [N_{PMD},R_{FPA}]	-	i/o	lv1a and lv1b/PQE store	**MDR-1*-Earthshine** PCD_EARTH F_BAD_STOKES 1 = bad 0 = OK or not checked

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
F_{cloud}	Flag indicating whether effective fractional cloud is greater than a specified threshold	bool	-	i/o	lv1a and lv1b/PQE store	**MDR-1*-Earthshine** PCD_EARTH_1BF_CLOUD 1 = above threshold 0 = below threshold

5.5.2.3.5 EXTRACT SELECTED MEASUREMENTS PER READOUT FOR "QUICK LOOK" PRODUCTS (A5.1.5): Input from Initialisation Data

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
λ_s^{331}	Start wavelength for window at approximately 331 nm	d	nm	i/o	PQE ini / 24 hour store	
λ_e^{331}	End wavelength for window at approximately 331 nm	d	nm	i/o	PQE ini / 24 hour store	
λ_s^{318}	Start wavelength for window at approximately 318 nm	d	nm	i/o	PQE ini / 24 hour store	
λ_e^{318}	End wavelength for window at approximately 318 nm	d	nm	i/o	PQE ini / 24 hour store	
λ^R	Wavelength for selecting 'Red' PMD	d	nm	i/o	PQE ini / 24 hour store	
λ^B	Wavelength for selecting 'Blue' PMD	d	nm	i/o	PQE ini / 24 hour store	
λ^G	Wavelength for selecting 'Green' PMD	d	nm	i/o	PQE ini / 24 hour store	
λ_s^{665}	Start wavelength for window at approximately 665 nm	d	nm	i/o	PQE ini / 24 hour store	
λ_e^{665}	End wavelength for window at approximately 665 nm	d	nm	i/o	PQE ini / 24 hour store	
λ_s^{780}	Start wavelength for window at approximately 780 nm	d	nm	i/o	PQE ini / 24 hour store	
λ_e^{780}	End wavelength for window at approximately 780 nm	d	nm	i/o	PQE ini / 24 hour store	

5.5.2.3.6 Input from VIADRs in Level 1b Product

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
SMR	Solar Mean Reference spectrum	d[D,B]	photons/(s.cm^2.sr.nm)	i/o	lv1b / 24 hour store	**VIADR-SMR** SMR *Only if SunNorm = AbsRad* *Only for* $(\lambda_s^{331} \le \lambda_i \le \lambda_e^{331})$ $(\lambda_s^{318} \le \lambda_i \le \lambda_e^{318})$ $(\lambda_s^{665} \le \lambda_i \le \lambda_e^{665})$ $(\lambda_s^{780} \le \lambda_i \le \lambda_e^{780})$

5.5.2.3.7 Input from VIADRs in Level 1b Product

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
Mode	Observation mode	enum	-	i/o	lv1b / 24 hour store	**MDR-1*** OBSERVATION_MODE
pmd_transfer	PMD transfer mode	enum	-	i/o	lv1b / 24 hour store	**MDR-1*** PMD_TRANSFER
longitude *latitude*	Geocentric longitude corresponding to actual integration time, ground, points ABCD (earth-fixed CS)	d[4]	degree		lv1b / 24 hour store	**MDR-1b-Earthshine** GEO_EARTHCORNER_ACTUAL For integration times greater than 187.5 ms, only the first *M* entries of the second dimension will be filled, where *M* is the number of readouts for that integration time.
θ	Satellite zenith angle	d[R_{FPA},3]	degree	i/o	lv1b / 24 hour store	**MDR-1*Earthshine** GEO_EARTHSAT_ZENITH
θ_0	Solar zenith angle	d[R_{FPA},3]	degree	i/o	lv1b / 24 hour store	**MDR-1*-Earthshine** GEO_EARTHSOLAR_ZENITH

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
S_{cal}	Signal detector readouts corrected for the radiance response of the instrument	d[D,B]	photons/(s.cm^2.sr.nm)	i/o	lv1b / 24 hour store	**MDR-1b-Earthshine** BAND_*RAD *Only if* *SunNorm = AbsRad* *Only for* $(\lambda_s^{331} \le \lambda_i \le \lambda_e^{331})$ $(\lambda_s^{318} \le \lambda_i \le \lambda_e^{318})$ $(\lambda_s^{665} \le \lambda_i \le \lambda_e^{665})$ $(\lambda_s^{780} \le \lambda_i \le \lambda_e^{780})$
R	Sun-normalised radiance or reflectivity	d[D,B]	-	i/o	lv1b / 24 hour store	**MDR-1b-Earthshine** BAND_*RAD *Only if* *SunNorm = AbsRad* *Only for* $(\lambda_s^{331} \le \lambda_i \le \lambda_e^{331})$ $(\lambda_s^{318} \le \lambda_i \le \lambda_e^{318})$ $(\lambda_s^{665} \le \lambda_i \le \lambda_e^{665})$ $(\lambda_s^{780} \le \lambda_i \le \lambda_e^{780})$

5.5.2.4 Algorithm

All data listed in Section 5.5.2.3 is extracted from the Level 1a and Level 1b product and made available to Process Product Quality Information (A5.2).

5.5.2.4.1 Update PQE Storage Location (A5.1.1)

All header data, global PCDs, PCDs extracted from VIADRs, and PCDs applicable per scan, as specified in Section 5.5.2.3, are written to the PQE storage location. The selected set of measurements required for the generation of "Quick Look" parameters as described in *Extract Selected Measurements per Readout for "Quick Look" Products* (A5.1.5) are stored for a period of twenty- four hours only.

5.5.3 PROCESS PRODUCT QUALITY INFORMATION (A5.2)

Input:

Product header information, PCDs both on a global and scan basis, PCDs providing information about the quality of applied calibration parameters and a selected sub-set of Earthshine measurements for calculation of "Quick-Look" information..

Output:

Product Quality Summaries and Daily "Quick-Look" information.

Uses Generic Sub-Functions:

None.

Uses Auxiliary Sub-Functions:

None.

Data Granule

One Product

5.5.3.1 Objectives

The data extracted by PQE Extraction (A5.1) are further condensed to provide daily, weekly, monthly and yearly Product Quality Summaries. Daily "Quick-Look" products are also generated. The highest level of detail, on measurement pixel level, is not covered by automatic PQE functionality.

5.5.3.2 Description

The data extracted by PQE Extraction (A5.1) comprises PCDs both on a product and scan level, and PCDs providing information about the quality of applied calibration parameters. Data is further condensed to provide daily, weekly, monthly and yearly Product Quality Summaries. "Quick-Look" products are also produced on a daily basis from a sub-set of Earthshine measurements and stored as colour maps. The PQE storage location will store Product Quality data for the lifetime of the mission and make it available for visualisation and analysis.

5.5.3.3 Variables

All variables specified in Section 5.5.2.3 are input to this module.

5.5.3.4 Algorithm

5.5.3.4.1 Generate Daily Quick-Look Data (A5.2.1)

The PQE storage location is accessed once per day to retrieve a selected set of measurements per detector readout as described in "Extract Selected Measurements per Readout for "Quick Look "Products (A5.1.5)" from all products sensed in the preceding twenty four hours.

5.5.3.4.2 Calculate Ozone Line Ratio (A5.2.1.1)

If *Mode* is equal to any of the Earth observation modes as defined in Section 5.2.5, then for *i* such that $\lambda_s^{331} \le \lambda_i \le \lambda_e^{331}$ and $\lambda_s^{318} \le \lambda_i \le \lambda_e^{318}$

If *SunNorm* = *AbsRad* extract $S_{Cal}(\lambda_i)$ and $SMR(\lambda_i)$ and calculate:

$$R^{331} = \sum_{i=\lambda_s^{331}}^{\lambda_e^{331}} S_{Cal}(\lambda_i) / \sum_{i=\lambda_s^{331}}^{\lambda_e^{331}} SMR(\lambda_i) \text{ and } R^{318} = \sum_{i=\lambda_s^{318}}^{\lambda_e^{318}} S_{Cal}(\lambda_i) / \sum_{i=\lambda_s^{318}}^{\lambda_e^{318}} SMR(\lambda_i)$$

Equation 247

or alternatively if *SunNorm* = *NormRad* extract $R(\lambda_i)$ and calculate:

$$R^{331} = \sum_{i=\lambda_s^{331}}^{\lambda_e^{331}} R(\lambda_i) \text{ and } R^{318} = \sum_{i=\lambda_s^{318}}^{\lambda_e^{318}} R(\lambda_i)$$

Equation 248

Then calculate for each ground pixel:

$$O_3LR = \frac{1}{(\sec\theta_{Sat,F} + \sec\theta_{Sun,F})} \cdot \frac{R^{331}}{R^{318}}$$

Equation 249

where $\theta_{Sat,F}$ and $\theta_{Sun,F}$ are the satellite zenith angle and the solar zenith angle appropriate to the centre of the ground pixel, point F, see *Calculate Geolocation for Fixed Grid (A2.6).*

5.5.3.4.3 Generate Data for False Colour Image (A5.2.1.2)

If *Mode* is equal to any of the *Earth* observation modes as defined in Section 5.2.5, and *pmd_transfer* = *band* + *raw* or *pmd_transfer* = *band* + *mixed* then for those PMD data in band mode extract the three PMD bands which contain or are closest to the wavelengths λ^R, λ^G and λ^B . These data will be used to generate a false colour image.

5.5.3.4.4 CALCULATE PROXY FOR NDVI AND NEAR INRA-RED WINDOW (A5.2.1.3)

If Mode is equal to any of the *Earth* observation modes as defined in Section 5.2.5, then for *i* such that $\lambda_s^{665} \le \lambda_i \le \lambda_e^{665}$ and $\lambda_s^{780} \le \lambda_i \le \lambda_e^{780}$ extract $S_{cal}(\lambda_i)$ and $SMR(\lambda_i)$. Alternatively, if *SunNorm* = *NormRad* extract $R(\lambda_i)$

If *SunNorm* = *AbsRad* extract $S_{cal}(\lambda_i)$ and $SMR(\lambda_i)$ and calculate:

$$R^{780} = \sum_{i=\lambda_s^{780}}^{\lambda_e^{780}} S_{Cal}(\lambda_i) / \sum_{i=\lambda_s^{780}}^{\lambda_e^{780}} SMR(\lambda_i) \text{ and } R^{665} = \sum_{i=\lambda_s^{665}}^{\lambda_e^{665}} S_{Cal}(\lambda_i) / \sum_{i=\lambda_s^{665}}^{\lambda_e^{665}} SMR(\lambda_i)$$ *Equation 250*

or alternatively if *SunNorm* = *NormRad* extract $R(\lambda_i)$ and calculate

$$R^{665} = \sum_{i=\lambda_s^{665}}^{\lambda_e^{665}} R(\lambda_i) \text{ and } R^{780} = \sum_{i=\lambda_s^{780}}^{\lambda_e^{780}} R(\lambda_i)$$ *Equation 251*

Then for each ground pixel, calculate NDVI = 1n(R^{665} / R^{780}) and

$$IRWin = R^{780}$$ *Equation 252*

5.5.3.4.5 Plot 'Quick-Look' Data on Global Map (A5.2.1.4)

The 'Quick Look' data are plotted once per day, using the geolocation information, on a global colour map and the plots stored in the PQE data store in a suitable graphics format for the lifetime of the mission.

5.5.3.4.6 Generate Product Quality Summaries (A5.2.2)

For any specified time interval (daily, weekly, monthly, yearly) retrospective product quality information, specifically all Header information, global PCDs, PCDs extracted from VIADRs and PCDs applicable per scan, as described in Section 5.5.2.3, shall be retrieved from the Product Quality storage location.

For the specified time period the following information shall be calculated and stored in Product Quality Summaries:

1. Summary header information indicating start UTC times, end UTC times, Product Identifier range, and algorithm or status flags for in-flight calibration data included in the summary.
2. The sum of each global PCD describing an occurrence number
3. The mean of each global PCD describing a mean quantity
4. The sum of occurrences of non-nominal flags contained in VIADR PCDs
5. The sum of each VIADR PCD describing an occurrence number

6. The mean of each VIADR PCD describing a mean quantity
7. The sum of occurrences of non-nominal flags contained in PCDs applicable to scans
8. The sum of PCDs applicable to scans describing an occurrence number
9. The mean of PCDs applicable to scans describing a mean quantity

The generated Product Quality Summaries shall be stored in the PQE storage location and made available for visualisation and analysis in time-series plots and simple statistical analysis.

5.6 VISUALISATION (A6)

5.6.1 Overview

The Visualisation functionality shall provide all the imaging facilities required for the visualisation of the GOME-2 science data packets, level 0, 1a and 1b products including in-flight calibration data and correction factors. It shall also support the visualisation of the quality information produced by the PQE functionality, and monitoring information produced by the SPA functionality.

The visualisation functionality shall comprise time series visualisation, spectra visualisation and map visualisation. Time-series visualisation provides a time-series of any word or parameter to be selected by the user. A text description of the content of the word or parameter shall also be provided. In the case of Level 0, 1a or 1b products time series of mean signals per band or individual detector pixel readouts shall both be possible. Spectra visualisation shall provide a plot of the whole spectrum measured per channel. Map visualisation shall provide data on maps, including a display comprising two maps with different scales, one of them indicating the orbit and the other displaying a colour-coded diagram with the value of the measurements along the orbit.

In addition the visualisation functionality shall provide a manual interface via an HMI to facilitate user interaction thereby allowing selection of the type of visualisation to be performed and selection of the specific data and parameters to be displayed. At the highest level the HMI should offer the user the selection of products or data for visualisation. The data selected will remain available in memory until the user exits or resets the session. The selection of more than one dataset for visualisation shall be possible. It shall be possible to view the product header of the selected data on request. A pop-up text box shall appear on the screen with the requested information.

5.6.2 SDP, Level 0, 1A and 1B product visualisation (A6.1)

For the visualisation of GOME-2 science data packets, level 0, 1a and 1b products following visualisation capabilities are required.

5.6.2.1 Time Series Visualisation (A6.1.1)

For time series visualisation the y-axis shall represent the parameter value and x-axis the succession of data packets. In addition when more than one dataset is selected the two datasets shall be superimposed on the same plot for simple comparison. Selected housekeeping data for provision of information about each data packet shall be appended to the interface for user information. Furthermore, each dataset shall be clearly labelled for identification of each dataset. A paging facility shall be available in order to progress through the previously selected words (“Back” and “Next”). Statistical data shall be available automatically for each visualised dataset including at least minimum, maximum, mean and standard deviation. In order to provide information for the user regarding the precise data values which are being displayed on the screen, an interactive information display shall be provided with the data values corresponding to each dataset. This shall be activated with an “Interactive On/Off” button. Further, a “view value” key shall be provided that permits the user written inspection of values displayed on screen. It shall also be possible to dump this report to a file.

5.6.2.2 Spectra Visualisation (A6.1.2)

The spectra visualisation functionality allows display of a complete spectrum organised into channels, namely the four main FPA channels and the two PMD channels. The screen shall be divided into different areas such that all channels can be visualised at one time. On the right-hand side, information about the position of the spectra within the ISP sequence shall be available. A “go-to” key shall be provided for rapid display of a selected packet without stepping through all previous packets. Statistical data shall be available automatically for each visualised dataset including at least minimum, maximum, mean and standard deviation.

5.6.2.3 Map Visualisation (A6.1.3)

The map visualisation functionality shall provide one global map displaying the orbit and a second presenting the colour-coded data in its geographical position. The data available for display on the map shall be the same as those displayed in the time-series. The user shall be able to select the data for visualisation and step backwards and forwards along the orbit.

5.6.3 IN-FLIGHT CALIBRATION DATA VISUALISATION (A6.2)

In-flight calibration data comprise both spectra and single parameter data. Selection of parameters shall be possible via an interactive menu. Where appropriate spectra visualisation shall be made available as described in Section 5.6.2.2. In the case of in-flight calibration data where data is sorted on the basis of other parameters (e.g. dark signal correction) it shall be possible to navigate through the complete set of data. Correction factors input to the GOME-2 level 0 to 1a processor shall also be visualised via the spectra visualisation functionality as described in Section 5.6.2.2.

5.6.4 SPA AND PQE VISUALISATION (A6.3)

For quality information generated by the PQE functionality as described in Section 5.5, both the time series and map visualisation functionality shall be made available as described in Section 5.6.2.1 and Section 5.6.2.3. For monitoring information generated by the SPA functionality as described in Section 5.4, all of time series, spectra and map visualisation functionality shall be made available as described in Section 5.6.2.1, Section 5.6.2.2 and Section 5.6.2.3.

5.7 GENERIC PROCESSING SUB-FUNCTIONS

5.7.1 Initialise Orbit Propagator (AG.1)

Uses Generic Sub-Functions:

PGE services providing geolocation parameters will be used.

Uses Auxiliary Sub-Functions:

None.

Data Granule

Orbit state vector. Typically once per orbit.

5.7.1.1 Objectives

Ensure that the PGE orbit propagator is correctly initialised for the current orbit state vector.

5.7.1.2 Description

The details of processing depend on the actual implementation and interfaces of the PGE services for orbit propagation. For the purpose of this description, the following is assumed (see variable list below for details):

- There will be an orbit propagator (called `mo_orbit` below) which allows accurate prediction of osculating Cartesian and Kepler state vectors for user requested times.
- The orbit propagator can be run in two modes, initialisation and propagation. A proper sequence of orbit propagator calls consists of one initialisation call and a number of propagation calls. This module performs the initialisation call. See module Calculate Geolocation for Fixed Grid (A2.6) for the propagation calls.
- An osculating Cartesian orbit state vector (UTC; position and velocity in earth-fixed coordinate system) at or near (± 5° latitude) true (earth-fixed) ascending node crossing is available on input. This allows propagation over a complete orbit. The ascending node crossing epoch of this state vector must fall within two orbital periods of the user requested UTC time in the sub-sequent propagation calls.
- When run in initialisation mode the orbit propagator calculates accurate values for the Mean Kepler elements at the true (earth-fixed) ascending node in true-of-date coordinates.
- The orbit propagator can be run in a high accuracy mode where the latitude and longitude-dependent geo ID anomalies as well as a medium air drag and luni-solar perturbations are accounted for.

It is anticipated that the initialisation mode of the orbit propagator will be run once per orbit at a time which would be dependent upon the availability of the initial osculating state vector. This state vector can then be fed into the propagator in order to initialize the propagation.

5.7.1.3 Variables

The variable names used in the `mo_orbit` routine are indicated in italics in the References/Remarks column.

5.7.1.3.1 Input from orbit dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
t_0	UTC of initial osculating state vector (processing format): fractional days after 1 Jan 2000 ΔUT1 = UT1–UTC	d[2]	[day][s]	i	A2.0.2	*mjdp* assumed to be zero
x_0	Initial Cartesian osculating position vector (earth-fixed CS)	d[3]	m	i	A2.0.2	*pos*
v_0	Initial Cartesian osculating velocity vector (earth-fixed CS)	d[3]	m/s	i	A2.0.2	*vel*

5.7.1.3.2 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
t_{ANX}	UTC of the true ascending node (processing format)	d[2]	[day][s]	o	A2.6	*mjdr*
K_{ANX}	Mean Kepler elements at the true ascending node (true-of-date CS): Semi-major axis Eccentricity Inclination Argument of perigee Mean anomaly Right ascension of ascending node	d[6]	[m] [–] [deg] [deg] [deg] [deg]	o		*xm*

5.7.1.4 Algorithm

This module is a wrapper for the call to the orbit propagator in initialisation mode. It passes the input parameters to the orbit propagator and returns the output specified above from the orbit propagator.

The *mode* parameter of `mo_orbit` is chosen as follows:

$$mode = \mathrm{MO\_INIT} + \mathrm{MO\_NO\_RESULTS} \quad \textit{Equation 253}$$

In this way the orbit propagator is initialised for longitude dependent calculations and does not produce any optional results. The initial state vector (x_0, v_0) has to be within 5° of latitude near the ascending node crossing, and t_0 within two nodal periods from the requested UTC time in the sub-sequent propagation calls. The error introduced by setting ΔUT1 to zero can be neglected.

Details on error handling are implementation specific and cannot be given here. However, the out-put status of the PGE orbit propagator shall be checked, and appropriate measures taken in the event of errors.

5.7.2 CALCULATE GEOLOCATION FOR FIXED GRID (AG.2)

Instrument Modes		Instrument Data	
Earth	√	PMD	
Dark	√	FPA	
Sun	√	Housekeeping	√
WLS	√		
SLS	√		
SLS over Diffuser	√		
LED	√		
Moon	√		
Other	√		

Uses Generic Sub-Function:

PGE services providing geolocation parameters will be used.
Initialise Orbit Propagator (AG.1)
Calculate Centre Coordinates (AG.20)

Uses Auxiliary Sub-Functions:

None

Data Granule

One scan.

5.7.2.1 Objectives

Calculate a set of geolocation parameters (depending on the instrument mode) from an orbit state vector, the UTC, and scanner viewing angles.

5.7.2.2 Description

This module provides an accurate mapping from the GOME frame coordinates (UTC and viewing angle) to earth-fixed ground pixel coordinates (latitude, longitude) and solar and line-of-sight azimuth and zenith angles. The actual set of geolocation parameters to be calculated depends on the GOME measurement mode.

For space and time coordinates, the conventions given in Appendix C shall be followed.

It is assumed that the orbit propagator has been initialised using module Initialise Orbit Propagator (AG.1) for the current orbit before this module is called.

Most geolocation parameters are calculated in granules of the shortest effective integration time for the main channels (187.5 ms, R_{FPA} = 32 times per scan), independent of the actual integration time in the main channels. In the case of PMD geolocation the parameters are also calculated for the shortest integration time (23.375 ms, R_{PMD} = 256 times per scan). The remaining geolocation parameters are calculated once per scan, either because their variation within a scan is small, or because they are not needed on a finer grid by higher-level processing (e.g., sub-satellite point coordinates).

5.7.2.2.1 BASIC AND MODE SPECIFIC GEOLOCATION PARAMETERS

A common basic set of geolocation parameters is calculated for all measurement modes. This includes the latitude and longitude of the sub-satellite point (SSP), and the solar zenith and azimuth angles at the satellite. For the earth observation, sun and moon modes, additional parameters specific to these modes are calculated:

- For earth observation measurements, solar and line-of-sight zenith and azimuth angles at a given top-of-atmosphere height, the corner and centre coordinates of the ground pixel at ground level, the satellite height, and the earth radius are calculated.
- For solar measurements, the distance between satellite and sun and the relative speed of satellite and sun are calculated.
- For lunar measurements, a number of parameters describing the lunar measurement geometry are calculated.

All geolocation calculations expect on input an orbit state vector (mean Kepler elements at true ascending node crossing) and the time for which the calculation shall be performed. In addition, the calculations for earthshine measurements need the scanner viewing angles and the size of the instantaneous field-of-view (IFOV).

5.7.2.2.2 PROCESSING STEPS

The exact sequence of processing steps depends on which geolocation parameters can be retrieved together from a call to the PGE services. For the purpose of this description, the following is assumed (see variable lists below for details):

- There will be an orbit propagator module providing longitude and latitude of the sub-satellite point and the apparent sun radius as seen from the satellite. This module is called `mo_orbit` in the following.
- The orbit propagator can be run in two modes, initialisation and propagation. A proper sequence of orbit propagator calls consists of one initialisation call and a number of propagation calls. This module performs the propagation calls. See the module *Initialise Orbit Propagator (AG.1)* for the initialisation call.

- There will be a pointing module providing all target related geolocation parameters, in particular elevation and azimuth angles. This module is called *mp_target* in the following.
- The pointing module can be run in a mode where it calculates only the directions to the sun and the moon, and in a mode where it calculates in addition the first intersection point of the line of sight with a surface at a given altitude above the earth's surface.

The general sequence of processing steps is as follows:

1. AG.2.1: Determine sub-satellite point (`mo_orbit` calls).
2. AG.2.2 Calculate line-of-sight azimuth and elevation angles for the ground footprint.
3. AG.2.3: Calculate target pointing information (`mp_target` calls).

The detailed sequence of processing steps depends on the instrument mode. In calibration (except sun/moon) and other modes only the basic set of geolocation parameters is calculated. The following processing steps are required:

1. Determine sub-satellite point, i.e., its geodetic latitude and geocentric longitude in the earth-fixed CS.
2. (not required)
3. Calculate target pointing information for the sun, i.e., solar zenith and azimuth angles in the Satellite Relative Actual CS.

The processing steps for measurements in **sun** and **moon** mode are as follows:

1. Determine sub-satellite point and the distance between the satellite and the sun.
2. (not required)
3. Calculate target pointing information for the sun and moon.

The processing steps for measurements in **earth observation** mode with its extended set of geolocation parameters are as follows:

1. Determine sub-satellite point.
2. For the ground footprint, calculate line-of-sight azimuth and elevation angles in the Satellite Relative Actual CS. These are intermediate results not reported in the product, but needed as input for step 3.
3. Calculate target pointing information for earth and sun.

The PGE services may provide output parameters in addition to those requested. However, the variable lists below specify only those parameters needed for further processing.

5.7.2.3 Variables

The variables are listed per processing step. Capital letters are used to denote azimuth (ϕ) and elevation (*E*) angles in the Satellite Relative Actual Reference CS, while small letters are used for azimuth (φ) and elevation (e) angles in the topocentric CS (at top-of-atmosphere).

5.7.2.3.1 Determine sub-satellite point (AG.2.1)

5.7.2.3.1.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
i	Cartesian coordinate	i	-	t	-	0…2
k	Index number of current scan mirror readout within scan	i	-	t	-	0…$R_\phi - 1$ (R_ϕ) *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*
n	Index number of current 187.5 ms ground pixel within scan, or in the case of PMD data the index number of 23.4375 ms readout within a scan.	i	-	t	-	0…$R_{FPA} - 1$ *or* 0…$R_{PMD} - 1$

5.7.2.3.1.2 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
R_{Sun}	Semi-diameter of the sun	d	m	i	A2.0.1	

5.7.2.3.1.3 Input from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
mode	Observation mode	enum	m	i	A2.0.1	
t_ϕ	UTC corresponding to scanner viewing angle with additional element at end of scan	d[R_ϕ +1]	days	i	A2.3.2, A3.2.2	*In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
t_{ANX}	UTC of the true ascending node (processing format)	d[2]	days	i	AG.1	*mjdrmjdr*
K_{ANX}	Mean Kepler elements at the true ascending node (true-of-date CS): Semi-major axis Eccentricity Inclination Argument of perigee Mean anomaly Right ascension of ascending node	d[6]	 m – degree degree degree degree	i	AG.1	*xm*

5.7.2.3.1.4 Local Variables

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
ρ_{Sun}	Apparent semi-diameter of the sun	d[R_{FPA}]	degree	t	-	*res*[21]. Only first and last element will be used.

5.7.2.3.1.5 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
x_{Sat}	Satellite position (earth-fixed CS)	d[R_ϕ+1,3]	m	o	AG.2.3	*pos* *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*
v_{Sat}	Satellite velocity (earth-fixed CS)	d[R_ϕ+1,3]	m/s	o	AG.2.3	*vel* *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
a_{Sat}	Satellite acceleration (earth-fixed CS)	d[R_{ϕ}+1,3]	m/s2	o	AG.2.3	*acc* *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*
t_{geo}	UTC time corresponding to every second scanner position i.e., for *k* = 0, 2,…, 60, 62 (R_{FPA} = 32 times per scan)	d[R_{FPA}]	days	o	A2.23.1	**MDR-1*** GEO_BASICUTC_TIME
lon_{Sat}	Geocentric longitude of the satellite and SSP (earth-fixed CS)	d[R_{FPA}]	degree	o	A2.23.1	**MDR-1*** GEO_BASICSUB_SATELLITE_POINT *res*[7]
lat_{Sat}	Geodetic latitude of the satellite and SSP (earth-fixed CS)	d[R_{FPA}]	degree	o	A2.23.1	**MDR-1*** GEO_BASICSUB_SATELLITE_POINT *res*[8]
h_{Sat}	Geodetic altitude of the satellite (earth-fixed CS)	d[R_{FPA}]	m	o	A2.23.1	**MDR-1*** GEO_BASICSATELLITE_ALTITUDE *res*[27]
$D_{Sat-Sun}$	Distance between satellite and sun	d	m	o	A2.23.1	**MDR-1*-Sun** GEO_SUNDISTANCE_SAT_SUN Sun mode only
$v_{Sat-Sun}$	Relative speed of satellite and sun (negative if satellite is moving towards the sun)	d	m/s	o	A2.20.4, A2.23.1	**MDR-1*-Sun** GEO_SUNVEL_SAT_SUN Used in Doppler shift calculations (AG.19) Sun mode only
R_{Earth}	Earth radius at SSP (earth-fixed CS)	d	m	o	A2.23.1	**MDR-1*-Earthshine** GEO_EARTHEARTH_RADIUS Earth mode only

5.7.2.3.2 CALCULATE LINE-OF-SIGHT ANGLES FOR THE GROUND FOOTPRINT (AG.2.2)

5.7.2.3.2.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Index number of current scan mirror readout within scan	i	-	t	-	$0 \ldots R_\psi - 1$ (R_ψ) *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*
n	Index number of current 187.5 ms ground pixel within scan for FPA data, or index number of 23 ms ground pixel within scan for PMD data.	i	-	t	-	$0 \ldots R_{FPA}-1$ or $0 \ldots R_{PMD}-1$ Relation to *k:* see below.
m	Point within ground pixel	i	-	t	-	0…6, corresponding to A…G in this order. Letters A…G will be used below.

5.7.2.3.2.2 Local Variables

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
δ_ψ	Across-track LOS offset angle with respect to the IFOV centre	d	degree	t	-	
δ_y	Along-track LOS offset angle with respect to the IFOV centre	d	degree	t	-	

5.7.2.3.2.3 Input from key data set

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$IFOV_\psi$	Across-track (dispersion direction) instantaneous field of view	d	degree	i	A2.0.4	
$IFOV_y$	Along-track (cross-dispersion direction) instantaneous field of view	d	degree	t	A2.0.4	

5.7.2.3.2.4 Input from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
mode	Observation mode	enum	-	i	A2.3.1, A3.2.2	
ψ	Scanner viewing angle with additional element at end of scan	$d[R_\psi+1]$	degree	i	A2.3.1, A3.2.2	

5.7.2.3.2.5 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
ϕ	LOS azimuth angles, points A-G (Satellite Relative Actual Reference CS)	$d[R_{FPA},7]$ or $d[R_{PMD},7]$	degree	o	AG.2.3	
E	LOS elevation angles, points A-G (Satellite Relative Actual Reference CS)	$d[R_{FPA},7]$ or $d[R_{PMD},7]$	degree	o	AG.2.3	

5.7.2.3.3 CALCULATE TARGET POINTING INFORMATION (AG2.3)

The corresponding variable names used in the mp_target routine are indicated in italics in the References/Remarks column.

5.7.2.3.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
i	Cartesian coordinate	i	-	t	-	
k	Index number of current scan mirror readout within scan	i	-	t	-	$0 \ldots R\psi$ *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*
n	Index number of current 187.5 ms ground pixel within scan for FPA data, or index number of 23 ms ground pixel within scan for PMD data.	i	-	t	-	$0 \ldots R_{FPA} - 1$ or $0 \ldots R_{PMD} - 1$

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
m	Point within ground pixel	i	-	t	-	0…6, corresponding to A…G in this order. Letters A…G will be used below.

5.7.2.3.3.2 Local Variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
h_T	Target height	d	m	t	-	*dir*[2] 0 or h_0
mjdp	`mp_target` UTC time of calculation (processing format)	d[2]	days s	t	-	Absolute UTC
iatt	`mp_target` attitude control flag	i		t	-	*iatt* Assume 3 (yaw-steering mode)
aocs	`mp_target` AOCS parameters	d[3]	degree	t	-	*aocs* Dummy, assume 0.0
att	`mp_target` mispointing angles	d[3]	degree	t	-	*att* Assume 0.0
datt	`mp_target` mispointing rates	d[3]	degree/s	t	-	*datt* Assume 0.0
idir	`mp_target` direction mode switch	i			-	*idir*
dir	`mp_target` direction parameters For *idir* = MP_INTER_1ST: [0] LOS azimuth [1] LOS elevation [2] Target altitude [3]-[7] (treat as dummy) For *idir* = MP_GENERIC_TARG: [0] - [2] Target position (earth-fixed CS) [3] - [7] (treat as dummy)	d[8]	t degree degree m m	t	-	*dir*
ieres	`mp_target` extended results vector switch	i			-	*ieres*

t

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
E_{Sun}	Solar elevation (Satellite Relative Actual Reference CS)	d[R_{FPA}] *or* d[R_{PMD},3]	degree	t	-	*res*[54] All modes
e_{Sat}	Satellite elevation, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* [R_{PMD},3]	degree	t	-	*res*[9] Earth mode only
e_{Sun}	Solar elevation, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or*d[R_{PMD},3]	degree	t	-	*res*[67] Earth mode only
x_{Sun}	Sun position (earth-fixed CS)	d[3]	m	t	-	Moon mode only
x_{Moon}	Moon position (earth-fixed CS)	d[3]	m	t	-	Moon mode only
$x_{\text{Sun-Moon}}$	Vector from moon to sun (earth-fixed CS)	d[3]	m	t	-	Moon mode only
$x_{\text{Sat-Moon}}$	Vector from moon to satellite (earth-fixed CS)	d[3]	m	t	-	Moon mode only
$u_{\text{Sun-Moon}}$	Unit vector from moon to sun (earth-fixed CS)	d[3]	-	t	-	Moon mode only
$u_{\text{Sat-Moon}}$	Unit vector from moon to satellite (earth-fixed CS)	d[3]	-	t	-	Moon mode only
u_1	Unit vector orthogonal to $u_{\text{Sun-Moon}}$ and $u_{\text{Sat-Moon}}$	d[3]	-	t	-	Moon mode only
u_2	Unit vector orthogonal to $u_{\text{Sun-Moon}}$ and u_1	d[3]	-	t	-	Moon mode only
u_3	Unit vector orthogonal to $u_{\text{Sat-Moon}}$ and u_1	d[3]	-	t	-	Moon mode only
x	Cartesian coordinates of lunar points HJKLM (earth-fixed CS)	d[5,3]	m	t	-	Moon mode only

5.7.2.3.3.3 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
h_0	Height at which satellite and solar elevation and azimuth angles in the topocentric CS are calculated	d	m	i	A2.0.1	
$\Theta_{\text{Sun,Refr}}$	Solar zenith angle (Satellite Relative Actual Reference CS) threshold for change of `mp_target` ray tracing model switch	d	degree	i	A2.0.1	
$iray_{\text{Sun-Moon}}$	`mp_target` ray tracing model switch for calculation of solar/lunar angles in the Satellite Relative Actual Reference CS	i	-	i	A2.0.1	*iray*
$iray_{\text{Earth-LowSZA}}$	`mp_target` ray tracing model switch for calculation of topocentric parameters in earth observation mode for solar zenith angles below $\Theta_{Sun,Refr}$	i	-	i	A2.0.1	*iray*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$iray_{\text{Earth-HighSZA}}$	`mp_target` ray tracing model switch for calculation of topocentric parameters in earth observation mode for solar zenith angles above $\Theta_{Sun,Refr}$	i	-	i	A2.0.1	*iray*
freq	`mp_target` frequency of the signal	d	Hz	i	A2.0.1	*freq*
R_{Moon}	Semi-diameter of the moon	d	m	i	A2.0.1	

5.7.2.3.3.4 Input from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
mode	Observation mode	enum	-	i	A2.3.1	
t_ψ	UTC corresponding to scanner viewing angle with additional element at end of scan	$d[R_\psi + 1]$	days	i	A2.3.2, A3.2.2	*In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*
x_{Sat}	Satellite position (earth-fixed CS)	$d[R_\psi + 1,3]$	m	i	AG.2.1	*pos* *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*
v_{Sat}	Satellite velocity (earth-fixed CS)	$d[R_\psi+1,3]$	m/s	i	AG.2.1	*vel* *In the case PMD geolocation this is high resolution interpolated scan angle grid with 512 points.*
a_{Sat}	Satellite acceleration (earth-fixed CS)	$d[R_\psi+1,3]$	m/s2	i	AG.2.1	*acc* *In the case of PMD geolocation this is the high resolution interpolated scan angle grid with 512 points.*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
ϕ	LOS azimuth angles, points A-G (Satellite Relative Actual Reference CS)	$d[R_{FPA},7]$ *or* $d[R_{PMD},7]$	degree	i	AG.2.2	Earth mode only
E	LOS elevation angles, points A-G (Satellite Relative Actual Reference CS)	$d[R_{FPA},7]$ *or* $d[R_{PMD},7]$	degree	i	AG.2.2	

5.7.2.3.3.5 Input from static auxiliary dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
NE_{lat}	Number of latitudes in elevation dataset	i	-	i	A2.0.3	
NE_{lon}	Number of longitudes in elevation dataset	i	-	i	A2.0.3	
E_{lat}	Latitude grid for *Elev*	$d[NE_{lat}]$	degrees	i	A2.0.3	
E_{lon}	Longitude grid for *Elev*	$d[NE_{lat}]$	degrees	i	A2.0.3	
Elev	Elevation	$d[NE_{lat}, NE_{lon}]$	m	i	A2.0.3	

5.7.2.3.3.6 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
ϕ_{Sun}	Solar azimuth (Satellite Relative Actual Reference CS)	d[RFPA]	degree	o	A2.23.1	**MDR-1*** GEO_BASICSOLAR_AZIMUTH_ANGLE *res[53]*
Θ_{Sun}	Solar zenith (Satellite Relative Actual Reference CS)	d[RFPA]]	degree	o	A2.23.1	**MDR-1*** GEO_BASICSOLAR_ZENITH_ANGLE All modes
slon	Geocentric longitude for complete scan, ground, points ABCDF (earth-fixed CS)	d[5]	degree	o	A2.23.1	**MDR-1*-Earthshine** GEO_EARTHSCAN_CORNER& SCAN_CENTRE Earth mode only.

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
slat	Geodetic latitude for complete scan, ground, points ABCDF (earth-fixed CS)	d[5]	degree	o	A2.23.1	**MDR-1*-Earthshine** GEO_EARTHSCAN_CORNER& SCAN_CENTRE Earth mode only
lon	Geocentric longitude, ground, points ABCDF (earth-fixed CS)	d[R_{FPA},5] *or* d[R_{PMD},5]	degree	o	A2.7, A2.23.1, A3.2.2 A3.17.1	**MDR-1*-Earthshine** GEO_EARTH CORNER & CENTRE Earth mode only *or* **MDR-1b** GEO_EARTH_ACTUALCORNER_ACTUA L &CENTRE_ACTUAL Earth mode PMD data only. *res[3]*
lat	Geodetic latitude, ground, points ABCDF (earth-fixed CS)	d[R_{FPA},5] *or* d[R_{PMD},5]	degree	o	A2.7, A2.23.1, A3.2.2 A3.17.1	**MDR-1*- Earthshine** GEO_EARTH CORNER & CENTRE Earth mode only *or* **MDR-1b** GEO_EARTH_ACTUALCORNER_ ACTUAL & CENTRE_ACTUAL Earth mode PMD data only. *res*[5]
φ_{Sun}	Solar azimuth, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	o	A2.7, A2.23.1, A3.2.2 A3.17.1	**MDR-1*- Earthshine** GEO_EARTH SOLAR_ AZIMUTH Earth mode only *or* **MDR-1b** GEO_EARTH_ACTUALSOLAR_AZIMUTH_ACTUAL Earth mode PMD data only. *res*[66]
θ_{Sun}	Solar zenith, h_0, EFG (topocentric CS)	d[R_{FPA},3] *or* d[R_{PMD},3]	degree	o	A2.7, A2.23.1, A3.2.2 A3.17.1	**MDR-1*- Earthshine** GEO_EARTHSAT_AZIMUTH Earth mode only *or* **MDR-1b** GEO_EARTH_ACTUALSAT_AZIMUTH_ACTUAL Earth mode PMD data only. *res*[8]

Symbol	***Descriptive Name***	***Type***	***Units***	***I/O***	***Source***	***Remarks***
θ_{Sat}	Satellite zenith, *h*0, EFG (topocentric CS)	$d[R_{FPA},3]$ *or* $d[R_{PMD},3]$	degree	o	A2.7, A2.23.1, A3.2.2	**MDR-1*-Earthshine** GEO_EARTHSCAT_ANGLE Earth mode only 0°…180°
Θ	Scattering angle, h_0, F (topocentric CS)	$d[R_{FPA}]$	degree	o	A2.7,A2.21	
H	Surface elevation, F	$d[R_{FPA}]$	m	o	A2.23.1	**MDR-1*-Earthshine** GEO_EARTH SURFACE_ELEVATION Earth mode only
φ_{Moon}	Azimuth of lunar points HJKLM (Satellite Relative Actual Reference CS)	d[5]	degree	o	A2.23.1	**MDR-1*-Moon** GEO_MOON LUNAR_AZIMUTH *res*[12] Moon mode only
E_{Moon}	Elevation of lunar points HJKLM (Satellite Relative Actual Reference CS)	d[5]	degree	o	A2.23.1	**MDR-1*-Moon** GEO_MOON LUNAR_ELEVATION *res*[13] Moon mode only
$D_{Sun\text{-}Moon}$	Distance between sun and moon	d	m	o	A2.23.1	**MDR-1*-Moon** GEO_MOON DISTANCE_SUN_ MOON Moon mode only
$D_{Sat\text{-}Moon}$	Distance between satellite and moon	d	m	o	A2.23.1	**MDR-1*-Moon** GEO_MOONDISTANCE_SAT_MOON Moon mode only
ω	Lunar phase angle (geometrical)	d	degree	o	A2.23.1	**MDR-1*-Moon** GEO_MOONLUNAR_PHASE Moon mode only
A_{Moon}	Illuminated fraction of lunar disc (sunlit moon area divided by total moon area as seen from the satellite)	d	-	o	A2.23.1	**MDR-1*-Moon** GEO_MOON LUNAR_FRACTION Moon mode only

5.7.2.4 Algorithm

5.7.2.4.1 Determine Sub-Satellite Point (AG.2.1)

Notes:

1. The orbit propagator must have been successfully initialised (AG.1) such that the epoch of the ascending node crossing t_{ANX} and the requested time for prediction t_P are within two nodal periods.
2. Latitude, longitude, and satellite height are calculated on a 187.5 ms grid synchronised with every second scanner position, i.e., for k = 0, 2,…, 60, 62 (R_{FPA} = 32 times per scan) or for the PMDs for k = 0, 2,…, 510, 512 (R_{PMD} = 256 times per scan). Sun-satellite distance and relative speed, and sunlit area of the moon vary only little during a scan, so only one value per scan is returned.
3. These are calculations of satellite parameters. The GOME-2 scanner viewing angles are not used in this step.
4. The UTC times corresponding to every second scanner position t_{geo} i.e., for k = 0, 2,…, 60, 62 (32 times per scan) are also reported in the basic geolocation record.

   Loop information: Calculations below are performed for n = 0…R_{FPA}–1.

   Call the orbit propagator `mo_orbit` with the following input parameters:

$$omode = \begin{cases} \text{MO\_PROPAG} + \text{MO\_ORBIT\_RES\_BAS} + \text{MO\_ORBIT\_RES\_AUX} & \text{(Sun/Moon mode)} \\ \text{MO\_PROPAG} + \text{MO\_ORBIT\_RES\_BAS} & \text{(other modes)} \end{cases}$$ *Equation 254*

$$mjdr = t_{ANX}$$ *Equation 255*

$$xm = K_{ANX}$$ *Equation 256*

$$mjdp_0 = t_{\psi,\,2n}$$ *Equation 257*

$$mjdp_1 = 0$$ *Equation 258*

For each call, assign results to $x_{Sat,2n,i}$, $v_{Sat,2n,i}$, $a_{Sat,2n,i}$, $lon_{Sat,n}$, $lat_{Sat,n}$, $h_{Sat,n}$ (i = 0, 1, 2), and in addition to $\rho_{Sun,n}$ in sun mode. Convert $lon_{Sat,n}$ to the ISO 6709 representation using equation (404) where needed (see Appendix C).

End of loop.

Now x_{Sat}, v_{Sat}, a_{Sat}, contain values for k = 0, 2,…, 60, 62. Fill the remaining elements by linear extrapolation and interpolation as follows:

$$x_{Sat,\,64,\,i} = x_{Sat,\,62,\,i} + x_{Sat,\,62,\,i} - x_{Sat,\,60,\,i} \quad (i = 0, 1, 2),$$ *Equation 259*

$$x_{Sat,k,i} = (x_{Sat,k-1,i} + x_{Sat,k+1,i})/2 \quad (k = 1, 3, \ldots, 63, i = 0, 1, 2),$$ *Equation 260*

and similarly for v_{Sat} and a_{Sat}.

Sun observation mode only: Using ρ_{Sun} from the first orbit propagator call (n = 0), calculate the distance between satellite and sun from the following:

$$D_{\text{Sat-Sun}} = \frac{180}{\pi} \cdot \frac{R_{\text{Sun}}}{\rho_{\text{Sun},0}}.$$ *Equation 261*

Using ρ_{Sun} from the first (n = 0) and last (n = 31) orbit propagator calls, calculate the relative speed of satellite and sun from this:

$$v_{\text{Sat-Sun}} = \frac{180}{\pi} \cdot \frac{R_{\text{Sun}}}{31 \cdot 187.5 \cdot 10^{-3}} \cdot \left(\frac{1}{\rho_{\text{Sun},31}} - \frac{1}{\rho_{\text{Sun},0}}\right)$$ *Equation 262*

which is the difference in distance divided by the difference in time (31 × 87.5 ms). It is important to perform this calculation in double precision as the difference in distance is small compared to the distance between satellite and sun (typically 40 km compared to 150 million km). As GOME-2 solar calibrations are performed at sunrise, i.e., with the satellite moving towards the sun, $v_{\text{Sat-Sun}}$ will be negative.

Earth observation modes only: Use R_{Earth} from the first orbit propagator call (n = 0) as earth radius.

5.7.2.4.2 Calculate Line-Of-Sight Angles for the Ground Footprint (AG.2.2)

These calculations are performed for the Earth observation mode only. Their purpose is to derive from the scanner viewing angle and the IFOV dimensions the LOS elevation and azimuth angles in the Satellite Relative Actual Reference CS. These angles are needed in the next step (Calculate Target Pointing Information) as input to the PGE services. They are not reported in the product.

Notes:

1. For FPAs, angles are calculated for 187.5 ms ground pixels (R_{FPA} = 32 times per scan). For PMDs angles are calculated for 23.4375 ms integration times (R_{PMD} = 256 times per scan).Ground pixel n (n running from 0 to $R_{FPA} - 1$ or 0 to $R_{PMD} - 1$) corresponds to the part of the scan from $k = 2n$ to $k = 2n + 2$.
2. For each ground pixel, angles are calculated for seven selected points, as shown in Figure 11, and detailed in Table 5. Points A to D are the corner coordinates of the ground pixel on ground. Points E to G are in the centre of the along-track IFOV, and at the top of the atmosphere.

3. Due to the across-track extension δ_ψ of the IFOV there will be a slight overlap between adjacent ground pixels. Therefore, in the forward scan, corner points CD of ground pixel *n* will be different from corner points AB of ground pixel *n* + 1. In the back scan, corner points AB of ground pixel *n* will be different from corner points CD of ground pixel *n* + 1.
4. These are pure geometrical calculations. The UTC is not used in this step.

Loop information: Calculations below are performed for all ground pixels ($n = 0 \ldots R_{FPA} - 1$ or $n = 0 \ldots R_{PMD} - 1$) and points within a ground pixel (*m* = A…G).

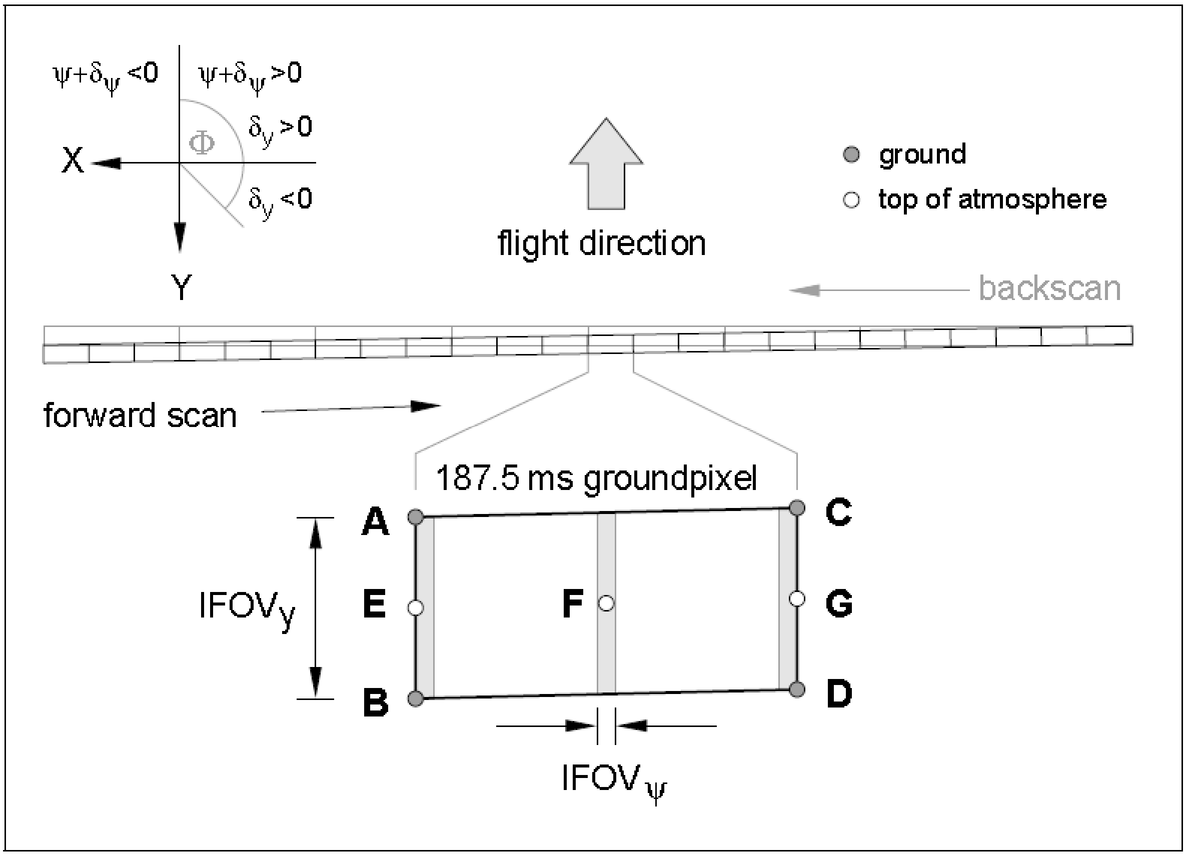

Figure 18: Ground pixel geometry for the level 0 to 1a processing. Directions X, Y, and line-of-sight azimuth angle ϕ refer to the Satellite Actual Reference Coordinate System. The orientation of the ground pixel points is the same for forward scan and back scan. The orientation of corner points ABCD is also used for the geolocation of the complete scan.

For a given ground pixel *n* and point *m*, assign values to scan mirror readout index *k* and LOS offset angles δ_ψ and δ_y according to Table 5. In order to have the points within the ground pixel always oriented the same way (AEB “left”, CGD “right”, see Figure 18), the selection of the scanner position depends on the scan direction of the current ground pixel as indicated in the table. For FPAs ground pixels $n = 0 \ldots 23$ are within the forward scan. Ground pixels $n = 24 \ldots 31$ belong to the back scan.

m	**A**	**B**	**C**	**D**	**E**	**F**	**G**
	left front	left aft	right front	right aft	left	centre	right
k (forward)	$2n$	$2n$	$2n+2$	$2n+2$	$2n$	$2n+1$	$2n+2$
k (backward)	$2n+2$	$2n+2$	$2n$	$2n$	$2n+2$	$2n+1$	$2n$
δ_y	$+IFOV_y/2$	$-IFOV_y/2$	$+IFOV_y/2$	$-IFOV_y/2$	0	0	0
δ_ψ	$-IFOV_\psi/2$	$-IFOV_\psi/2$	$+IFOV_\psi/2$	$+IFOV_\psi/2$	$-IFOV_\psi/2$	0	$+IFOV_\psi/2$
h_T (lat/lon)	0	0	0	0	N/A	0	N/A
h_T (elev/azim)	N/A	N/A	N/A	N/A	h_0	h_0	h_0

Table 5: Scan mirror indices, LOS offset angles and target heights. Scan mirror indices k (given for ground pixel n), LOS offset angles across track (δ_ψ) and along track (δ_y), and target heights h_T for ground pixel points A to G . Note that the time is implicitly given by the scan mirror index k.

The LOS elevation and azimuth angles in the Satellite Relative Actual Reference CS are then calculated from ψ_k, δ_ψ, and δ_y as follows: The LOS elevation angle is calculated from the following:

$$E_{nm} = \operatorname{asin}(\cos(\psi_k + \delta_\psi)\cos\delta_y), \quad -90° \le E_{nm} \le 90°$$ *Equation 263*

and the LOS azimuth angle (see also Figure 18) is given by the following:

$$\phi_{nm} = \begin{cases} 90° \text{ if } (\psi_k + \delta_\psi) \ge 0 \text{ and } \delta_y = 0 \\ 270° \text{ if } (\psi_k + \delta_\psi) < 0 \text{ and } \delta_y = 0 \\ 0 \text{ if } (\psi_k + \delta_\psi) = 0 \text{ and } \delta_y > 0 \\ 180° \text{ if } (\psi_k + \delta_\psi) = 0 \text{ and } \delta_y < 0 \\ \operatorname{atan}\dfrac{\sin(\psi_k + \delta_\psi)\cos\delta_y}{\sin\delta_y} \text{ otherwise } \begin{pmatrix} 0 < \phi_{nm} < 180° \text{ if } (\psi_k + \delta_\psi) > 0 \\ 180° < \phi_{nm} < 360° \text{ if } (\psi_k + \delta_\psi) < 0 \end{pmatrix} \end{cases}$$ *Equation 264*

Notes:

1. For the equation $\psi_k + \delta_\psi = 0$ and $\delta_y = 0$ and while looking in –Z (nadir) direction, the azimuth angle is actually not defined, but we set it to be 90°.
2. The atan operation shall be implemented using a function similar to the C maths library function `atan2 (y,x)` which returns atan (y/x) in the range $-\pi$ to $+\pi$. Compared to the `atan` function, `atan2` has the advantage that its range of values covers 360° as required. However, as we follow the convention of having azimuth angles between 0 and 360°, 360° has to be added to the result of the `atan2` operation if it is negative (which occurs if and only if $\psi_k + \delta_\psi < 0$).
3. For the coordinates of the ground pixel centre point F we have $\delta\psi = \delta_y = 0$, which reduces equation (263) and equation (264) to the following:

$$E_{nF} = 90° - |\psi_k|$$ *Equation 265*

and

$$\phi_{n\mathrm{F}} = \begin{cases} 90° \text{ if } \psi_k \geq 0 \\ 270° \text{ if } \psi_k < 0 \end{cases}$$ *Equation 266*

End of loop.

5.7.2.4.3 Calculate Target Pointing Information (AG.2.3)

Calculations to be performed depend on the instrument mode.

All modes:

Solar azimuth ϕ_{Sun} and solar zenith angle Θ_{Sun} in the Satellite Relative Actual Reference CS are part of the basic geolocation record which is calculated for all measurement modes.

Loop information: Calculations below are performed for all ground pixels ($n = 0 \ldots R_{FPA}-1$).

Call target pointing routine mp_target with the following input parameters (see Variable List above for remaining input parameters) where $k = 2n + 1$:

$$mjdp_0 = t_{\psi, k}$$ *Equation 267*

$$mjdp_1 = 0$$ *Equation 268*

$$pos_i = x_{Sat, k, i} \quad (i = 0, 1, 2)$$ *Equation 269*

$$vel_i = v_{Sat, k, i} \quad (i = 0, 1, 2)$$ *Equation 270*

$$acc_i = a_{Sat, k, i} \quad (i = 0, 1, 2)$$ *Equation 271*

$$idir = \text{MP\_NO\_TAR (no target point)}$$ *Equation 272*

$$dir_i = 0 \quad (i = 0, 1, 2) \text{ (dummy input)}$$ *Equation 273*

$$ieres = \text{MP\_TARG\_RES\_SAT2SUN}$$ *Equation 274*

$$iray = iray_{\mathrm{SunMoon}}$$ *Equation 275*

For each call, assign results to $\phi_{Sun,n}$ and $E_{Sun,n}$.

Convert solar elevation $E_{Sun,n}$ to the solar zenith $\Theta_{Sun,n}$ using Equation 403 in Appendix C.

End of loop.

5.7.2.4.4 Earth observation modes:

Loop information: Calculations below are performed for all ground pixels ($n = 0 \ldots R_{FPA} - 1$ or $n = 0 \ldots R_{PMD} - 1$) and points within a ground pixel (m = A…G).

For a given ground pixel n and point m, assign values to scan mirror readout index k and target height h_T according to Table 5. Note that for centre point F, `mp_target` has to be called twice: once with $h_T = 0$ for the latitude/longitude calculations, and once with $h_T = h_0$ for both the elevation azimuth calculations.

Call target pointing routine `mp_target` with the following input parameters (see Variable List above for remaining input parameters):

$$mjdp_0 = t_{\psi, k}$$ *Equation 276*

$$mjdp_1 = 0$$ *Equation 277*

$$pos_i = x_{Sat, k, i} \quad (i = 0, 1, 2)$$ *Equation 278*

$$vel_i = v_{Sat, k, i} \quad (i = 0, 1, 2)$$ *Equation 279*

$$acc_i = a_{Sat, k, i} \quad (i = 0, 1, 2)$$ *Equation 280*

idir = MP_INTER_IST (find first intersection point of LOS with surface at height h_T) *Equation 281*

$$dir_0 = \phi_{nm} \text{ (target azimuth)}$$ *Equation 282*

$$dir_1 = E_{nm} \text{ (target elevation)}$$ *Equation 283*

$$dir_2 = h_T \text{ (target height)}$$ *Equation 284*

$$ieres = \begin{cases} \text{MP\_TARG\_RES\_SAT2TARG} & (m = \text{A, B, C, D}) \\ \text{MP\_TARG\_RES\_SAT2TARG} + \text{MP\_TARG\_RES\_TARG2SUN} & (m = \text{E, F, G}) \end{cases}$$ *Equation 285*

$$iray = \begin{cases} iray_{\text{EarthLowSZA}} \text{ if } \Theta_{\text{Sun}, n} \le \Theta_{\text{Sun, Refr}} \\ iray_{\text{EarthHighSZA}} \text{ if } \Theta_{\text{Sun}, n} > \Theta_{\text{Sun, Refr}} \end{cases}$$ *Equation 286*

If m = A, B, C, D ($h_T = 0$): Assign results to ground pixel corner coordinates lon_{nm}, lat_{nm}.
If m = F ($h_T = 0$): Assign results to ground pixel centre coordinates lon_{n4}, lat_{n4}.

If m = E, F, G ($h_T = h_0$): Assign results to satellite and solar elevation and azimuth angles:

$\varphi_{Sat,n,m-4}$

$e_{Sat,n,m-4}$

$\varphi_{Sun,n,m-4}$

$e_{Sun,n,m-4}$

See variable list for corresponding elements of the `mp_target` results vector.

Convert the longitude *lon* to the ISO 6709 representation using equation (404) where needed (see Appendix C).
Convert the satellite and solar elevation e_{Sat} and e_{Sun} to the satellite and solar zenith θ_{Sat} and θ_{Sun} using Equation 405 in Appendix C.

Calculate the cosine of the scattering angle for the central point F as follows:

$$\cos\Theta_n = -\cos\theta_{Sat,nF}\cos\theta_{Sun,nF} + \sin\theta_{Sat,nF}\sin\theta_{Sun,nF}\cos(\varphi_{Sat,nF} - (\varphi_{Sun,nF} + 180°)) \quad \text{Equation 287}$$

and the scattering angle itself by applying the acos function on cos Θ_n (range of values 0…180°).
Θ is defined in the interval 0…180°, and the sign convention is such that $\Theta = 0$ for forward scattering, and $\Theta = 180°$ for backward scattering. $\theta_{Sat} = 0$ for overhead satellite and $\theta_{Sun} = 0$ for overhead sun at scattering point, in accordance with the section on topocentric coordinate systems in Appendix C.

Using an external database for surface elevation, find the surface elevation H_n of the (latitude/longitude) grid element which contains the latitude and longitude coordinates lon_{n4}, lat_{n4} of the ground pixel centre point F.

End of loop.

Finally, the geolocation of the complete scan is derived by selecting the appropriate coordinates from the individual 187.5 ms ground pixels for the four corner points ABCD:

$$slat_A = lat_{31,A}, slon_A = lon_{31,A} \quad \text{Equation 288}$$

$$slat_B = lat_{0,B}, slon_B = lon_{0,B} \quad \text{Equation 289}$$

$$slat_C = lat_{24,C}, slon_C = lon_{24,C} \quad \text{Equation 290}$$

$$slat_D = lat_{24,D}, slon_D = lon_{24,D} \quad \text{Equation 291}$$

Determine the (approximate) scan centre point F by a call to module Calculate Centre Coordinates (AG.20), providing coordinates of points B and C, $slon_B$, $slat_B$, $slon_C$, $slat_C$, on input. The module will return centre coordinates $slon_F$, $slat_F$ on output.

Lunar mode:

Note: Lunar parameters are calculated for the start of the scan only ($k = 0$).
Below we use vector notation as follows: Let $\boldsymbol{x}$, $\boldsymbol{y}$ be cartesian vectors with components x_i, y_i ($i = 0, 1, 2$). Then their sum (difference) is calculated per component, the product (ratio) with a scalar is calculated per component, their dot product is defined as follows:

$$x \bullet y = \sum_{i=0}^{2} x_i y_i$$

Equation 292

their vector product as:

$$x \times y = \begin{pmatrix} x_1 y_2 - x_2 y_1 \\ x_2 y_0 - x_0 y_2 \\ x_0 y_1 - x_1 y_0 \end{pmatrix}$$

Equation 293

and their cartesian length as:

$$|x| = \sqrt{x \bullet x}.$$

Equation 294

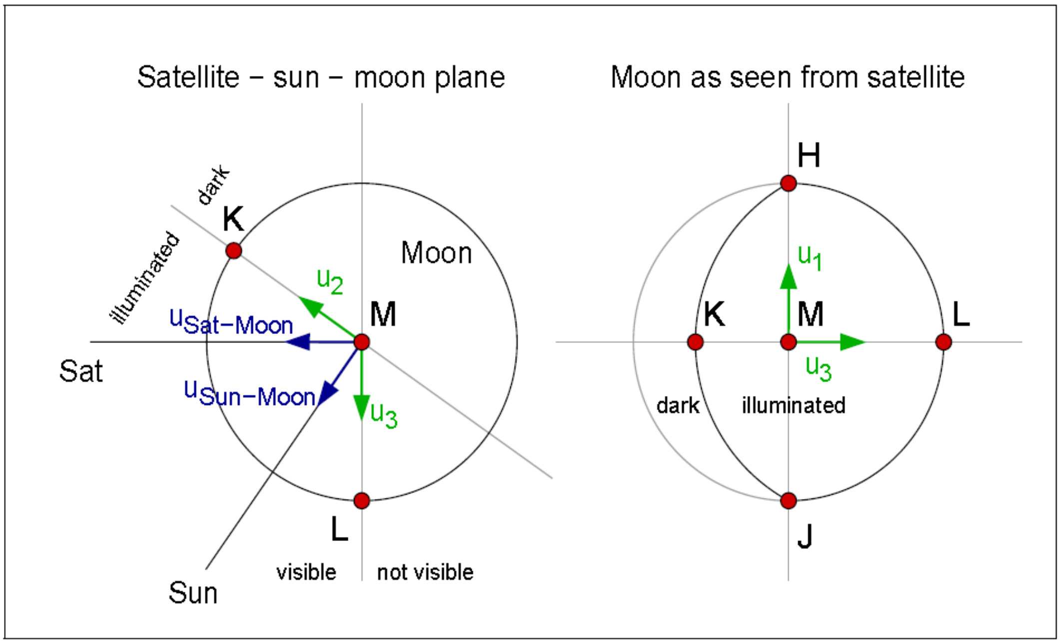

Figure 19: Geometry for lunar observations. Elevation and azimuth angles in the Satellite Relative Actual Reference CS are calculated for the four points HJKL delimiting the illuminated part of the lunar surface as seen from the satellite, and for point M, the centre of the moon.

Get positions of sun and moon in the true-of-date CS at time $t_{\psi,0}$ from PGE functions `ml_sun` and `ml_moon` respectively. Convert them from true-of-date to earth-fixed coordinates x_{Sun}, x_{Moon}, using PGE function `ml_change_sv_cs` with time $t_{\psi,0}$ on input.

Calculate the difference vectors

$$x_{\text{Sun-Moon}} = x_{\text{Sun}} - x_{\text{Moon}} \quad \text{Equation 295}$$

and

$$x_{\text{Sat-Moon}} = x_{\text{Sat, 0}} - x_{\text{Moon}} \quad \text{Equation 296}$$

and their cartesian lengths

$$D_{\text{Sun-Moon}} = \left| x_{\text{Sun-Moon}} \right| \quad \text{Equation 297}$$

and

$$D_{\text{Sat-Moon}} = \left| x_{\text{Sat-Moon}} \right| \quad \text{Equation 298}$$

Normalise the difference vectors to unit length:

$$u_{\text{Sun-Moon}} = x_{\text{Sun-Moon}} / D_{\text{Sun-Moon}}$$ *Equation 299*

$$u_{\text{Sat-Moon}} = x_{\text{Sat-Moon}} / D_{\text{Sat-Moon}}$$ *Equation 300*

Calculate a unit vector orthogonal to both of them:

$$u_1 = \frac{u_{\text{Sat-Moon}} \times u_{\text{Sun-Moon}}}{\left| u_{\text{Sat-Moon}} \times u_{\text{Sun-Moon}} \right|}$$ *Equation 301*

a unit vector orthogonal to $u_{\text{Sun-Moon}}$ and u_1:

$$u_2 = u_{\text{Sun-Moon}} \times u_1$$ *Equation 302*

and a unit vector orthogonal to $u_{\text{Sat-Moon}}$ and u_1:

$$u_3 = u_1 \times u_{\text{Sat-Moon}}$$ *Equation 303*

The illuminated fraction of the lunar disc A_{Moon} (as seen from the satellite) is given by:

$$A_{Moon} = (1 + u_{\text{Sat-Moon}} \bullet u_{\text{Sun-Moon}}) / 2$$ *Equation 304*

The lunar phase angle ω is calculated from:

$$\omega = \begin{cases} \operatorname{acos}(u_{\text{Sat-Moon}} \bullet u_{\text{Sun-Moon}}) & \text{if } u_{12} < 0 \\ -\operatorname{acos}(u_{\text{Sat-Moon}} \bullet u_{\text{Sun-Moon}}) & \text{if } u_{12} \geq 0 \end{cases}$$ *Equation 305*

ω is defined here as the geometrical (!) angle between the direction from the moon to the sun and the direction from the moon to the satellite. It is (close to) 0 for full moon and (close to) ±180° for new moon, negative for waxing moon, positive for waning moon. The range of values of the acos function is assumed to be from 0 to 180°. u_{12} is the Z component of vector u_1.

The earth-fixed coordinates of the points HJKL on the lunar surface and the moon centre M are defined by:

$$x_H = x_{\text{Moon}} + R_{\text{Moon}} u_1$$ *Equation 306*

$$x_J = x_{\mathrm{Moon}} - R_{\mathrm{Moon}} u_1$$ *Equation 307*

$$x_K = x_{\mathrm{Moon}} + R_{\mathrm{Moon}} u_2$$ *Equation 308*

$$x_L = x_{\mathrm{Moon}} + R_{\mathrm{Moon}} u_3$$ *Equation 309*

$$x_M = x_{\mathrm{Moon}}$$ *Equation 310*

Loop information: The following calculations are performed for the five lunar points m = H, J, K, L, M.

Call target pointing routine `mp_target` with the following input parameters (see Variable List above for remaining input parameters):

$$mjdp_0 = t_{\psi,0}$$ *Equation 311*

$$mjdp_1 = 0$$ *Equation 312*

$$pos_i = x_{Sat,0,i} \quad (i = 0, 1, 2)$$ *Equation 313*

$$vel_i = v_{Sat,0,i} \quad (i = 0, 1, 2)$$ *Equation 314*

$$acc_i = a_{Sat,0,i} \quad (i = 0, 1, 2)$$ *Equation 315*

$$idir = \mathrm{MP\_GENERIC\_TARG} \text{ (target point given by its earth-fixed coordinates)}$$ *Equation 316*

$$dir_i = x_{mi} \quad (i = 0, 1, 2) \text{ (earth-fixed coordinates of target point)}$$ *Equation 317*

$$dir_i = 0 \quad (i = 3, 4, 5) \text{ (rates are not needed here)}$$ *Equation 318*

$$ieres = \mathrm{MP\_TARG\_RES\_SAT2TARG} \text{ (calculate basic satellite to target parameters)}$$ *Equation 319*

$$iray = iray_{\mathrm{SunMoon}}$$ *Equation 320*

Assign resulting satellite to target azimuth to lunar azimuth $\varphi_{Moon,m}$ and satellite to target elevation to lunar elevation $E_{Moon,m}$.

End of loop.

5.7.3 Calculate MMEs for PMD Data In Band Transfer Mode (AG.3)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

Linear Interpolation (AX.2)

Data Granule

N/A

5.7.3.1 Objectives

Calculate PMD band averages of Müller matrix element.

5.7.3.2 Description

In the case of PMD data transferred in *band + mixed* or *band + raw* transfer modes MMEs and their errors which are band averaged should be used. In this case it is necessary to calculate the MMEs and their ratios as the mean value over the PMD bandwidth. Mean errors are also calculated as appropriate. This is done by integrating the MMEs in question over the wavelength range associated with each PMD band. These calculations need only be repeated if the PMD band definition or the spectral calibration of the PMD band measurements are changed.

5.7.3.3 Variables

5.7.3.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
j	PMD channel	i	-	t	-	*p.s*
k	PMD band	i	-	t	-	

5.7.3.3.2 Local Variables

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
s^{PMD}	Pixel number defining the start of a PMD band with respect to the raw PMD wavelength grid on which the MMEs have been interpolated	i[NP_{MD}]	-	t	-	
e^{PMD}	Pixel number defining the end of a PMD band with respect to the raw PMD wavelength grid on which the MMEs have been calculated	i[NP_{MD}]	-	t	-	
$\delta\lambda^{raw}$	Wavelength interval between points on the raw PMD spectral grid	i[NP_{MD}]	-	t	-	Here N_{PMD} refers to the number of spectral grid points in the raw PMD wavelength grid.

5.7.3.3.3 Input from initialisation dataset or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$N_{\psi f}$	Number of viewing angles for which the fine viewing angle grid is specified	w	-	i	A2.0.1, A3.0.4	**GIADR-1a-MME** MME_N_PSI_F
N_{ef}	Number of solar elevation angles for which the fine elevation angle grid is specified	w	-	i	A2.0.1, A3.0.4	**GIADR-1a-MME** MME_N_E_F
$N_{\varphi f}$	Number of solar azimuth angles for which the fine azimuth angle grid is specified	w	-	i	A2.0.1, A3.0.4	**GIADR-1a-MME** MME_N_PHI_F
Ψ_f	Viewing angles which define the fine viewing angle grid.	d[$N_{\phi f}$]	degree	i	A2.0.1, A3.0.4	**GIADR-1a-MME** MME_PSI_F

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
e_f	Solar elevation angles which define the fine elevation angle grid	d[N_{ef}]	degree	i	A2.0.1, A3.0.4	**GIADR-1a-MME** MME_E_F
φ_f	Solar azimuth angles which define the fine azimuth angle grid	d[$N_{\phi f}$]	degree	i	A2.0.1, A3.0.4	**GIADR-1a-MME** MME_PHI_F
N_{PMD}	Total number of PMD bands	w	-	i	A2.0.1, A3.0.4	

5.7.3.3.4 *Input from level 0 data stream and level 1a data stream*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
s	Pixel number defining the start of a PMD band	i[N_{PMD},2]	-	i	A2.0.7, A3.0.4	**MDR-1a*** ISP_HEAD
l	Length in pixels of a PMD band	i[N_{PMD},2]	-	i	A2.0.7, A3.0.4	**MDR-1a*** ISP_HEAD

5.7.3.3.5 *Input/output from other functions or level 1a data stream*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
λ^{MME}	Wavelength grid on which the Müller Matrix Elements are calculated	d[D,B]	-	i/o	A2.1, A3.0.4	**GIADR-1a-MME** MME_WL
M^1	Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D,B, $N_{\psi f}$]	BU.s^{-1}/(photons/(s.cm^2.s r.nm))	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_RAD_RESP
$M^{1,irrad}$	Müller matrix element describing the irradiance response of the instrument to unpolarised light	d[D,B, N_{ef}, $N_{\varphi f}$]	BU.s^{-1}/(photons/(s.cm^2.nm))	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_IRRAD_RESP
μ^2	Ratio of MMEs M^2 to M^1 describing the polarisation sensitivity of the instrument with respect to the Q Stokes component (s/p polarisation). Derived from key data parameter η.	d[D,B,$N_{\psi f}$]		i	A2.1, A3.0.4	**GIADR-1a-MME** MME_POL_SENS

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
μ^3	Ratio of MMEs M^3 to M^1 describing the polarisation sensitivity of the instrument with respect to the U Stokes component (+/–45° polarisation). Derived from key data parameter.	d[D,B,$N_{\psi f}$]		i	A2.1, A3.0.4	**GIADR-1a-MME** MME_POL_SHIFT
$M^1_{(s/p)}$	Response ratio of PMD-s/PMD-p as a function of viewing angle	d[D,$N_{\psi f}$]		i	A2.1, A3.0.4	**GIADR-1a-MME** MME_INT_RAT
ε_M^1	Relative error in the Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D,B]	-	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_ERR_RAD_RESP
$\varepsilon\_M^{1,irrad}$	Relative error in the Müller matrix element describing the irradiance response of the instrument to unpolarised light	d[D,B]	-	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_ERR_IRRAD_RESP
ε_μ^2	Relative error in the ratio of MMEs M^2 to M^1 which describes the polarisation sensitivity of the instrument with respect to the Q Stokes component	d[D,B]	-	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_ERR_POL_SENS
ε_μ^3	Relative error in the ratio of MMEs M^3 to M^1 which describes the polarisation sensitivity of the instrument with respect to the U Stokes component	d[D,B]	-	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_ERR_POL_SHIFT
$\varepsilon\_M^1_{SN}$	Relative error in the sun-normalised radiance response	d[D,B]	-	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_SNRR_ERR
λ^{raw}	Most recent raw PMD wavelength grid	d[D,N_{PMD}]	-		A2.15, A3.6	

5.7.3.3.6 Output: band averaged parameters

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$\overline{M^1}$	Müller matrix element describing the radiance response of the instrument to unpolarised light	$d[D,B,N_{\psi f}]$	$BU.s^{-1}/(photons/(s.cm^2.s\ r.nm))$	o	various	
$\overline{M^{1,irrad}}$	Müller matrix element describing the irradiance response of the instrument to unpolarised light	$d[D,B,N_{ef},N_{\varphi f}]$	$BU.s^{-1}/(photons/(s.cm^2.s\ r.nm))$	o	various	
$\overline{\mu^2}$	Ratio of MMEs M^2 to M^1 which describes the polarisation sensitivity of the instrument with respect to the Q Stokes component	$d[D,B,N_{\psi f}]$	-	o	various	
$\overline{\mu^3}$	Ratio of MMEs M^3 to M^1 which describes the polarisation sensitivity of the instrument with respect to the U Stokes component	$d[D,B,N_{\psi f}]$	-	o	various	
$\overline{M^1_{s/p}}$	Response ratio of PMD-s/PMD-p as a function of viewing angle	$d[D, N_{\psi f}]$	-	o	various	
$\varepsilon\_M^{1,irrad}$	Relative error in the Müller matrix element describing the irradiance response of the instrument to unpolarised light	d[D,B]	-	o	various	
$\overline{\varepsilon\_\mu^2}$	Relative error in the ratio of MMEs M^2 to M^1 which describes the polarisation sensitivity of the instrument with respect to the Q Stokes component	d[D,B]	-	o	various	
$\overline{\varepsilon\_\mu^3}$	Relative error in the ratio of MMEs M^3 to M^1 which describes the polarisation sensitivity of the instrument with respect to the U Stokes component	d[D	-	o	various	
$\overline{\varepsilon\_M^1}$	Relative error in the Müller matrix element describing the radiance response of the instrument to unpolarised light	d[D	-	o	various	
$\overline{\varepsilon\_M^1_{SN}}$	Relative error in the sun-normalised radiance response	d[D	-	o	various	

5.7.3.4 Algorithm

First interpolate the MMEs from the MME spectral grid λ^{MME} to the raw PMD-p or PMD-s spectral grid as appropriate λ^{raw} using Spline Interpolation (AX.3).

First for $k = 1...N_{PMD}$ calculate s_{jk}^{raw} and e_{jk}^{raw} for $j = p$ and $j = s$ such that:

$$\lambda^{raw}(s_{jk}^{raw}) = \lambda(s_{jk}) \text{ and } \lambda^{raw}(e_{jk}^{raw}) = \lambda(s_{jk} + l_{jk} - 1)$$ *Equation 321*

The integrals are estimated by discrete summation for $k = 1...N_{PMD}$, $j = p$ and $j = s$, $\psi = \psi_1...\psi_{N_\psi}$, $e = e_1...e_{N_e}$ and $\varphi = \varphi_1...\varphi_{N_\varphi}$ as:

$$\overline{M_{kj,\,\psi}^{1}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} M_{ij,\,\psi}^{1} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$ *Equation 322*

$$\overline{M_{kj,\,e\varphi}^{1,\,irrad}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} M_{ij,\,e\varphi}^{1,\,irrad} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$ *Equation 323*

$$\overline{\mu_{kj,\,\psi}^{2}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \mu_{ij,\,\psi}^{2} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$ *Equation 324*

$$\overline{\mu_{kj,\,\psi}^{3}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \mu_{ij,\,\psi}^{3} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$ *Equation 325*

$$\overline{M_{(s/p)k,\,\psi}^{1}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} M_{(s/p)i,\,\psi}^{1} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$ *Equation 326*

$$\overline{\varepsilon\_M_{kj}^{1}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \varepsilon\_M_{ij}^{1} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$

Equation 327

$$\overline{\varepsilon\_M_{kj}^{1,\,irrad}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \varepsilon\_M_{ij}^{1,\,irrad} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$

Equation 328

$$\overline{\varepsilon\_\mu_{kj}^{2}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \varepsilon\_\mu_{ij}^{2} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$

Equation 329

$$\overline{\varepsilon\_\mu_{kj}^{3}} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \varepsilon\_\mu_{ij}^{3} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$

Equation 330

$$\overline{\varepsilon\_M_{SN,\,kj}}^{1} = \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \varepsilon\_M_{SN,\,ij}^{1} \cdot \delta\lambda_i^{raw}\right) \Big/ \left(\sum_{i = s_{jk}^{MME}}^{e_{jk}^{MME}} \delta\lambda_i^{raw}\right)$$

Equation 331

Here if $i = s_{jk}^{raw} + 1 \ldots e_{jk}^{raw} - 1$:

$$\delta\lambda_i^{raw} = \frac{\lambda_{i+1}^{raw} - \lambda_{i-1}^{raw}}{2}$$

Equation 332

and

$$\delta\lambda_{s_{jk}^{MME}}^{raw} = (\lambda_{s_{jk}^{MME}+1}^{raw} - \lambda_{s_{jk}^{MME}}^{raw})/2 \text{ and } \delta\lambda_{e_{jk}^{MME}}^{raw} = (\lambda_{e_{jk}^{MME}}^{raw} - \lambda_{e_{jk}^{MME}-1}^{raw})/2$$

Equation 333

5.7.4 CONVERT HOUSEKEEPING DATA (AG.4)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.4.1 Objectives

Convert selected housekeeping data from instrument binary units into engineering units.

5.7.4.2 Description

This module converts selected GOME-2 housekeeping data from the raw instrument binary units into engineering units. Only those data which are relevant to the 0 to 1b processing are converted. These are (as a minimum) predisperser prism and detector temperatures, and lamp currents and voltages. For the conversion, polynomial coefficients from the GOME-2 TM/TC data sheets [AD6] have to be used. These coefficients have to be part of the initialisation dataset. Preliminary coefficients for use in processor testing are given in Appendix F.

5.7.4.3 Variables

5.7.4.3.1 Local Variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
k	Subset counter	i	-	t	-	*0…15*
m	Polynomial coefficient index	i	-	t	-	*0…4*
n	Selected HK data index	d[B]	-	t	-	*0…N–1*
t^{dt}	Detector temperature	d	K	t	-	
t^{pdp}	Pre-disperser prism temperature	d	K	t	-	
t^{rad}	Radiator temperature	d	K	t	-	
U^{SLS}	SLS lamp voltage	d	V	t	-	
I^{SLS}	SLS lamp current	d	A	t	-	
U^{WLS}	WLS lamp voltage	d	V	t	-	
I^{WLS}	WLS lamp current	d	A	t	-	

5.7.4.3.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
P_{nm}	Polynomial coefficients for HK conversion to engineering units	d[N,5]	(various)	i	A2.0.1	See [AD6].
ITTable	Integration times corresponding to indices 0…255 in the Science Data packet.	d[256]	s	i	A2.0.1	
T^{dt}_{low}	Lowest nominal detector temperature	d[B]	K	i	A2.0.1	
T^{dt}_{high}	Highest nominal detector temperature	d[B]	K	i	A2.0.1	
T^{pdp}_{low}	Lowest nominal pre-disperser prism temperature	d	K	i	A2.0.1	
T^{pdp}_{high}	Highest nominal predisperser prism temperature	d	K	i	A2.0.1	

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
T_{low}^{rad}	Lowest nominal radiator temperature	d	K	i	A2.0.1	
T_{high}^{rad}	Highest nominal radiator temperature	d	K	i	A2.0.1	
U_{low}^{SLS}	Lowest nominal SLS lamp voltage	d	V	i	A2.0.1	
U_{high}^{SLS}	Highest nominal SLS lamp voltage	d	V	i	A2.0.1	
I_{low}^{SLS}	Lowest nominal SLS lamp current	d	A	i	A2.0.1	
I_{high}^{SLS}	Highest nominal SLS lamp current	d	A	i	A2.0.1	
U_{low}^{WLS}	Lowest nominal WLS lamp voltage	d	V	i	A2.0.1	
U_{high}^{WLS}	Highest nominal WLS lamp voltage	d	V	i	A2.0.1	
I_{low}^{WLS}	Lowest nominal WLS lamp current	d	A	i	A2.0.1	
I_{high}^{WLS}	Highest nominal WLS lamp current	d	A	i	A2.0.1	
I_{on}^{WLS}	Minimum WLS current for the WLS to be considered “on”	d	A	i	A2.0.1	
I_{on}^{SLS}	Minimum SLS current for the SLS to be considered “on”	d	A	i	A2.0.1	

5.7.4.3.3 *Input from level 0 data stream*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
HK_{kn}	Selected housekeeping data in instrument units.	w[16,N]	BU	i	A2.0.7	**MDR_1a-***ISP_HEAD

Note: Subset of HK data actually converted is determined by the needs of the processor. See [AD9] for their location within HK. 16 data packets per scan, HK data are the first 488 words of a data packet, of which N are to be converted into engineering units.

5.7.4.3.4 *Global PCDs accumulated per product*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{nn_dt}	Number of scans with non-nominal detector temperature	w[B]				
N_{nn_pdp}	Number of scans with non-nominal pre-disperser prism temperature	w	-	g	A2.22	

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
N_{nn_rad}	Number of scans with non-nominal radiator temperature	w	-	g	A2.22	
N_{nn_WLSU}	Number of scans with non-nominal WLS lamp voltage	w	-	g	A2.22	
N_{nn_WLSI}	Number of scans with non-nominal WLS lamp current	w	-	g	A2.22	
N_{nn_SLSU}	Number of scans with non-nominal SLS lamp voltage	w	-	g	A2.22	
N_{nn_SLSI}	Number of scans with non-nominal SLS lamp current	w	-	g	A2.22	

5.7.4.3.5 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
$\breve{HK}_{kn}$	Selected housekeeping data converted to engineering units	d[16,N]	various	o	Further processing	
F_{nn_dt}	Flag indicating non-nominal detector temperature in scan	bool[B,R_{FPA}]	-	o	A2.23.1	**MDR-1a-***PCD_BASICF_NN_DT 1 = non-nominal 0 = nominal
F_{nn_pdp}	Flag indicating non-nominal pre-disperser prism temperature in scan	bool	-	o	A2.23.1	**MDR-1a-***PCD_BASICF_NN_PDP 1 = non-nominal 0 = nominal
F_{nn_rad}	Flag indicating non-nominal radiator temperature in scan	bool	-	o	A2.23.1	**MDR-1a-***PCD_BASICF_NN_RAD 1 = non-nominal 0 = nominal
F_{nn_WLSU}	Flag indicating non-nominal WLS voltage in scan	bool	-	o	A2.3.1 A2.23.1	**MDR-1a-***PCD_BASICF_NN_WLS_U 1 = non-nominal 0 = nominal
F_{nn_WLSI}	Flag indicating non-nominal WLS current in scan	bool	-	o	A2.3.1 A2.23.1	**MDR-1a-***PCD_BASICF_NN_WLS_I 1 = non-nominal 0 = nominal
F_{nn_SLSU}	Flag indicating non-nominal SLS voltage in scan	bool	-	o	A2.3.1 A2.23.1	**MDR-1a-***PCD_BASICF_NN_SLS_U 1 = non-nominal 0 = nominal
F_{nn_SLSI}	Flag indicating non-nominal SLS current in scan	bool	-	o	A2.3.1 A2.23.1	**MDR-1a-***PCD_BASICF_NN_SLS_I 1 = non-nominal 0 = nominal

5.7.4.4 Algorithm

5.7.4.4.1 Convert Housekeeping Data (AG.4.1)

Loop information: The following calculations are performed for all 16 data packets in the scan (k = 0...15)), and for all housekeeping data to be converted (n = 0...N – 1).

Convert housekeeping data from instrument units to engineering units using the following:

$$\hat{HK}_{kn} = \sum_{m=0}^{4} P_{nm} HK_{kn}^{m}$$ *Equation 334*

for housekeeping data except integration times, and

$$\hat{HK}_{kn} = ITTable_{HK_{kn}}$$ *Equation 335*

for integration times (main channels and PMD channels in calibration readout mode).

5.7.4.4.2 Calculate PCDs from Housekeeping Data (AG.4.2)

Initialise all flags to zero. If any of the flags below are raised the processing shall continue, a report shall be raised via the MCS and the products shall be flagged as degraded using the field DEGRADED_INST_MDR. Check temperatures as follows:

- For all detector temperatures recorded during each readout k of the scan, for j = 1...B if,

$$t_j^{dt} < t_{low,j}^{dt} \text{ or } t_j^{dt} > t_{high,j}^{dt} \text{ then}$$ *Equation 336*

$$F_{nn\_dt,\,jk} = 1 \text{ (stored for every readout)}$$ *Equation 337*

$$N_{nn\_dt,\,j} = N_{nn\_dt,\,j} + 1 \text{ (accumulated per channel and scan)}$$ *Equation 338*

- For all pre-disperser prism temperatures recorded during the scan, if

$$t^{pdp} < t_{low}^{pdp} \text{ or } t^{pdp} > t_{high}^{pdp} \text{ then}$$ *Equation 339*

$$F_{nn\_pdp} = 1$$ *Equation 340*

$$N_{nn\_pdp} = N_{nn\_pdp} + 1 \text{ (accumulated per scan)}$$ *Equation 341*

- For all radiator temperatures recorded during the scan, if

$$t^{rad} < t_{low}^{rad} \text{ or } t^{rad} > t_{high}^{rad} \text{ then}$$ Equation 342

$$F_{nn\_rad} = 1$$ Equation 343

$$N_{nn\_rad} = N_{nn\_rad} + 1$$ Equation 344

Radiator temperatures are passed to A2.23 to be included in the level 1a product in MDR-1a-* RAD_TEMP. Check lamp voltages and currents as follows:

- For all WLS voltages recorded during the scan, if

$$I^{WLS} > I_{on}^{WLS} \text{ and } (U^{WLS} < U_{low}^{WLS} \text{ or } U^{WLS} > U_{high}^{WLS}) \text{ then}$$ Equation 345

$$F_{nn\_WLSU} = 1$$ Equation 346

$$N_{nn\_WLSU} = N_{nn\_WLSU} + 1$$ Equation 347

- For all WLS currents recorded during the scan, if

$$I^{WLS} > I_{on}^{WLS} \text{ and } (I^{WLS} < I_{low}^{WLS} \text{ or } I^{WLS} > I_{high}^{WLS}) \text{ then}$$ Equation 348

$$F_{nn\_WLSI} = 1$$ Equation 349

$$N_{nn\_WLSI} = N_{nn\_WLSI} + 1$$ Equation 350

- For all SLS voltages recorded during the scan, if

$$I^{SLS} > I_{on}^{SLS} \text{ and } (U^{SLS} < U_{low}^{SLS} \text{ or } U^{SLS} > U_{high}^{SLS}) \text{ then}$$ Equation 351

$$F_{nn\_SLSU} = 1$$ Equation 352

$$N_{nn\_SLSU} = N_{nn\_SLSU} + 1$$ Equation 353

- For all SLS currents recorded during the scan, if

$$I^{SLS} > I_{on}^{SLS} \text{ and } (I^{SLS} < I_{low}^{SLS} \text{ or } I^{SLS} > I_{high}^{SLS}) \text{ then}$$ *Equation 354*

$$F_{nn\_SLSI} = 1$$ *Equation 355*

$$N_{nn\_SLSI} = N_{nn\_SLSI} + 1$$ *Equation 356*

5.7.5 PREPARE PMD DATA (AG.5)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.5.1 Objectives

Reconstruct PMD band signals by multiplying them with their co-adding factors.

5.7.5.2 Description

If GOME-2 uses PMD band transfer (as described in Appendix B), PMD readouts are spectrally co-added into 15 bands and divided by co-adding factors before they are transmitted to ground. The co-adding factors are selected such that the result fits into a 2-byte word. They are reported (as exponents to the base of 2) in the PMD status words of the Science Data Packet. This module reconstructs the PMD band signals by multiplying the signals in the Science Data Packet with their respective co-adding factors. This is the first processing step to be applied on PMD band data.

5.7.5.3 Variables

5.7.5.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
i	PMD band	i	-	t		*0…14*
j	PMD channel	i	-	t		*5…6*
k	PMD readout	i	-	t		*0…15*

5.7.5.3.2 Input from level 0 or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{jki}	PMD co-adding exponents	i[2,16,15]	-	i	A2.0.7, A3.0.4	**MDR-1a-***BAND_PPBAND_PS
S_{jki}	PMD band signals	w[2,16,15]	BU	i	A2.0.7, A3.0.4	**MDR-1a-***BAND_PPBAND_PS
l	Length in pixels of a PMD band	i[N_{PMD},2]	-		A2.0.7, A3.0.4	**MDR-1a***ISP_HEAD

5.7.5.3.3 Input/output from other functions or the level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
pmd_transfer	PMD transfer mode	enum	-	i	A2.3.3, A3.0.4	**MDR-1a***PMD_TRANSFER

5.7.5.3.4 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$\hat{S}_{jki}$	Reconstructed PMD band signals	i[2,16,15]	-	i	A2.3.3, A3.0.4	

5.7.5.4 Algorithm

For all PMD channels, bands, and readouts using band data transfer calculate:

$$\hat{S}_{jki} = 2^{N_{jki}} \cdot S_{jki} / l_{ij}$$ *Equation 357*

Band data transfer is used

- in transfer mode 1: in all subsets except the subset of the PMD reset,
- in transfer mode 2: in all subsets except the subset of the PMD reset, and for 12 readouts of the subset of the PMD reset.

For PMD data not using band data transfer nothing is done.

5.7.6 CHECK FOR SATURATED PIXELS (AG.6)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.6.1 Objectives

To check for detector pixel saturation on the basis of pre-specified threshold values supplied per channel as input.

5.7.6.2 Description

If a detector pixel read-out exceeds a certain limit specified in the initialisation dataset for each band, it is regarded as being saturated. A saturation mask is generated per band for each readout in the scan. Bands affected by saturation are excluded from further processing. Further, a flag is set per scan and band if saturated pixels are detected in any readout in the scan. Note that a saturation check may only be applied to PMD data transferred in raw mode. For PMD data transferred in *band + raw* or *band + mixed* mode nothing is done.

5.7.6.2.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Index number of 187.5 ms ground pixel in the scan	i	-	t	-	0… R_{FPA} – 1. Readout 0 is the first readout in the first data packet of the scan.

5.7.6.2.2 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
t_{sat}	Saturation threshold per band	d[B]	BU	i	A2.0.1	

5.7.6.2.3 Input from level 0 data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
pmd_transfer	PMD transfer mode	enum	-	i	A2.0.7	

5.7.6.2.4 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
pmd_transfer	PMD transfer mode	enum	-	o	A2.3.3	

5.7.6.2.5 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
satpix	Saturation mask per band	b[B, R_{FPA}]	-	o	A2.4	1 = no saturation 0 = saturation
Fsat	Saturated pixel flag per channel	bool[B, R_{FPA}]]	-	o	A2.4	1 = saturation 0 = no saturation

5.7.6.3 Algorithm

If *pmd_transfer* = raw (i.e. PMD data is transferred in raw mode) the saturation check is applied to both main and PMD channels. Otherwise the saturation check is applied to main channels only. Nothing is done for PMD channels.

It is assumed that the saturation mask and flag are initialised such that $satpix = 1$ and $F_{sat} = 0$.

For each effective integration time k in the scan, a saturation mask is generated such that for $i = 0 \ldots D_j - 1$, $j = 1 \ldots B$ if the following:

$$S_{ij} > t_{sat,\ j} \text{ for any detector pixel } i \text{ in band } j \text{ then}$$ *Equation 358*

$$satpix_{jk} = 0 \text{ and } F_{sat,\ jk} = 1$$ *Equation 359*

Note that only one value of F_{sat} is recorded per band for every readout. The saturation mask is given per band, not per detector pixel, as we will exclude a complete band from processing even if only a single detector pixel is saturated. This is because of unknown side effects of saturated pixels on neighbouring pixels in the detector array.

5.7.7 CHECK FOR HOT PIXELS (AG.7)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.7.1 Objectives

To generate a hot pixel mask on the basis of pre-specified threshold values supplied as input.

5.7.7.2 Description

Generation of a hot pixel mask is done on the basis of pixel intensity. A hot pixel threshold is pre-specified as one value per band. A pixel is discarded from the calibration processing if its value deviates from that of the neighbouring pixels by more than the threshold value. The neighbouring pixels at either side of the hot pixel are also discarded as they are likely to be affected due to crosstalk between adjacent pixels. A flag is set per band if hot pixels are detected in any of the readouts in the scan.

A hot pixel check is only applied to measurements in *Dark*, *WLS*, and *LED* calibration modes. For the PMD data, an additional prerequisite is that PMD data are transferred in raw mode. If they are not, the hot pixel check is applied in the main channels only.

5.7.7.3 Variables

5.7.7.3.1 *Indices*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Index number of 187.5 ms ground pixel in the scan	i	-	t	-	0…R_{FPA}–1. Readout 0 is the first readout in the first data packet of the scan.

5.7.7.3.2 *Input from initialisation dataset*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
t_{hot}	Hot pixel threshold for band	d[B]	BU	i	A2.0.1	

5.7.7.3.3 *Input from level 0 data stream*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
S	Detector readout values for which the hot pixel mask is being generated	d[D,B]	BU	i	A2.0.7	

5.7.7.3.4 *Input/output from other functions*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
pmd_transfer	PMD transfer mode	enum	-	i	A2.3.3	

5.7.7.3.5 *Output*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
hotpix	Hot pixel mask	b[D,B,R_{FPA}]	-	o	A2.4	1 = normal pixel 0 = hot pixel
Fhot	Hot pixel flag per band	bool[B,R_{FPA}]	-	o		1 = hot 0 = not hot

5.7.7.4 Algorithm

If *pmd_transfer* = *raw* (i.e. PMD data is transferred in raw mode) the hot pixel check is applied to both main and PMD channels. Otherwise the hot pixel check is applied to main channels only. Nothing is done for PMD channels.

For every effective integration time k in the scan, if a detector pixel intensity deviates from the mean intensity in the band by more than a pre-specified threshold, it and the neighbouring detector pixels are flagged as hot pixels. It is assumed that the hot pixel mask and hot pixel flag are initialised such that $hotpix = 1$ and $F_{hot} = 0$.

For $i = 1...D_j - 2$, $j = 1...B$ and $k = 0...R_{FPA}$

If

$$S_{ij} > \frac{S_{(i-1)j} + S_{(i+1)j}}{2} + t_{hot,j}$$ *Equation 360*

then

$$\begin{bmatrix} hotpix_{(i+1)j} = 0 \\ hotpix_{ij} = 0 \\ hotpix_{(i-1)j} = 0 \end{bmatrix}$$ *Equation 361*

and

$$F_{hot,jk} = 1$$ *Equation 362*

For the ends of each channel where neighbouring pixels do not exist the following equations apply:

$$\text{if } S_{0j} > S_{1j} + t_{hot,j} \text{ then } \begin{bmatrix} hotpix_{1j} = 0 \\ hotpix_{0j} = 0 \end{bmatrix}$$ *Equation 363*

$$\text{or if } S_{(D_j-1)j} > S_{(D_j-2)j} + t_{hot,j} \text{ then } \begin{bmatrix} hotpix_{(D_j-1)j} = 0 \\ hotpix_{(D_j-2)j} = 0 \end{bmatrix}$$ *Equation 364*

If either case is true $F_{hotjk} = 1$. Note that only one value of F_{hot} is recorded per band for every readout.

5.7.8 CHECK FOR SAA (AG.8)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.8.1 Objectives

To determine whether measured data lies in the SAA anomaly.

5.7.8.2 Description

The SAA region will be specified as a rectangular region in longitude and latitude. The check will be evaluated on a readout basis. Calibration mode data measured in the SAA will not be used in calibration processing.

5.7.8.3 Variables

5.7.8.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Index number of 187.5 ms ground pixel in the scan	i	-	t	-	$0 \ldots R_{FPA} - 1$. Readout is the first readout in the first data packet of the scan.

5.7.8.3.2 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
lon_{SAA}	SAA longitude range (min/max)	d[2]	degrees	i/o	A2.0.1	
lat_{SAA}	SAA latitude range (min/max)	d[2]	degrees	i/o	A2.0.1	

5.7.8.3.3 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
lon_{Sat}	Geocentric longitude of the satellite and SSP (earth-fixed CS)	d	degree	i	A2.6	
lat_{Sat}	Geodetic latitude of the satellite and SSP (earth-fixed CS)	d	degree	i	A2.6	

5.7.8.3.4 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
F_{SAA}	SAA flag	bit-string [32]	-	o	A2.7	1 = in SAA 0 = not in SAA

5.7.8.4 Algorithm

Assuming F_{SAA} has been initialised to zero, then the scan is in the SAA and $F_{SAA,k} = 1$ if for any effective integration time k in the scan, both of the following conditions are fulfilled:

$$lon_{SAA,0} \leq lon_{Sat} \leq lon_{SAA,1}$$
$$lat_{SAA,0} \leq lat_{Sat} \leq lat_{SAA,1}$$

Equation 365

5.7.9 CHECK FOR SUNGLINT (AG.9)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.9.1 Objectives

To set a flag per readout indicating a danger of sunglint effect for one or more ground pixels in the scan.

5.7.9.2 Description

Sunglint is a phenomenon that invalidates the calculation of air mass factors in level 2 processing and must be flagged during Level 0 to 1a Processing (A2). Sunglint is strongly dependent on the observing geometry. The flag simply indicates a geometrical possibility. Sunglint will be checked for scans assigned to one of the earth observation modes only, and only over water. The check is performed for the shortest effective integration time of the main channels (187.5 ms: R_{FPA} = 32 times per scan) independent of the actual integration time. Two thresholds for medium and high sunglint danger will be used. A scan will be flagged for sunglint, if thresholds are exceeded in any of the 32 ground pixels.

5.7.9.3 Variables

5.7.9.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Index number of 187.5 ms ground pixel in the scan	i	-	t	-	$0 \ldots R_{FPA} - 1$. Readout is the first readout in the first data packet of the scan.

5.7.9.3.2 Input from initialisation dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$t_{1,sunglint}$	Threshold for low sunglint risk	d	degree	i	A2.0.1	
$t_{2,sunglint}$	Threshold for high sunglint risk	d	degree	i	A2.0.1	

5.7.9.3.3 Input from static auxiliary set

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
NM_{lat}	Number of latitudes in Land Sea Mask	i	-	i	stat	
NM_{lon}	Number of longitudes in Land Sea Mask	i	-	i	stat	
M_{lat}	Latitude grid for *LSM*	$d[NM_{lat}]$	degree	i	stat	
M_{lon}	Longitude grid for *LSM*	$d[NM_{lon}]$	degree	i	stat	
LSM	Land Sea Mask	$d[NM_{lat}, NM_{lon}]$	-	i	stat	

5.7.9.3.4 Input/Output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
θ	Satellite zenith angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degree	i	A2.6	
θ_0	Solar zenith angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degree	i	A2.6	
φ	Satellite azimuth angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degree	i	A2.6	
φ_0	Solar azimuth angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degree	i	A2.6	
lon	Geocentric longitude, points ABCDF (earth-fixed CS)	d[R_{FPA}5]	degree	i	A2.6	
lat	Geodetic latitude, points ABCDF (earth-fixed CS)	d[R_{FPA}5]	degree	i	A2.6	

5.7.9.3.5 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
Fsunglint_risk	Flag indicating risk of sunglint per scan.	enum[R_{FPA}]	-	o	A2.7	
Fsunglint_high_risk	Flag indicating high risk of sunglint per scan	enum[R_{FPA}]	-	o	A2.7	

5.7.9.4 Algorithm

Initialise $F_{sunglint\_risk}$ and $F_{sunglint\_high\_risk}$ to *NoRisk*. For every effective integration time *k* in the scan perform the following checks:

Using the land-sea mask *LSM*, check whether the centre point F of the 187.5 ms ground pixel is contained in a bin covered (fully or partly) by water.

Note: For this *bin*, the preferred spatial resolution of the land-sea mask for this check is 0.1 degree × 0.1 degree. Proceed only if this is the case.

$$\text{If } |\theta - \theta_0| < t_{1,sunglint} \text{ and } ||\varphi - \varphi_0| - 180.0| < t_{1,sunglint} \text{ then } F_{sunglint\_risk,k} = LowRisk.$$

$$\text{If } |\theta - \theta_0| < t_{2,sunglint} \text{ and } ||\varphi - \varphi_0| - 180.0| < t_{2,sunglint} \text{ then } F_{sunglint\_high\_risk,k} = HighRisk.$$

5.7.10 CHECK FOR RAINBOW (AG.10) (AG.10)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.10.1 Objectives

To set a flag per readout indicating a danger of rainbow for one or more ground pixels in the scan.

5.7.10.2 Description

Rainbow is a phenomenon which may result in high polarisation above water clouds. As this may invalidate assumptions made in the interpolation of fractional polarisation parameters it must be flagged during Level 0 to 1a Processing (A2). Rainbow is strongly dependent on the observing geometry. The flag simply indicates a geometrical possibility. The actual presence of reflecting surface (water or clouds) is not checked. The check is evaluated for shortest effective integration time of the main channels (187.5 ms: R_{FPA} = 32 times per scan) independent of the actual integration time. Line of sight angles have been calculated previously in Calculate Geolocation for Fixed Grid (A2.6). This calculation is performed for scans assigned to one of the earth observation modes only.

5.7.10.3 Variables

5.7.10.3.1 *Indices*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Index number of 187.5 ms ground pixel in the scan	i	-	t	-	0…R_{FPA} – 1. Readout is the first readout in the first data packet of the scan.

5.7.10.3.2 *Input from initialisation dataset*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
ρ_1	Reference angle for rainbow check	d	degree	i	A2.0.1	
ρ_2	Angular limit for rainbow check	d	degree	i	A2.0.1	

5.7.10.3.3 *Input/Output from other functions*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
Θ	Scattering angle, h_0, point F (topocentric CS)	d[R_{FPA}]	degree	i	A2.6	

5.7.10.3.4 *Output*

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$F_{rainbow}$	Flag indicating danger of rainbow	bool[R_{FPA}]	-	o	A2.7	1 = risk 0 = no risk

5.7.10.4 Algorithm

Initialise $F_{rainbow}$ to zero. For every effective integration time k evaluate the rainbow check such that if:

$$|\Theta - \rho_1| < \rho_2 \text{ then } F_{rainbow,k} = 1$$ *Equation 366*

5.7.11 APPLY DARK SIGNAL CORRECTION (AG.11)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.11.1 Objectives

To correct all measurements for dark signal. To provide an updated South Atlantic Anomaly (SAA) flag per individual readout based on band 1A signals and derived during level 1a to 1b processing only.

5.7.11.2 Description

The dark signal correction is dependent on integration time, detector temperature, PMD transfer and PMD readout mode (see Section 5.2.10) therefore the dark signal correction appropriate to the measurement integration time, detector temperature, PMD transfer and PMD readout mode must be selected from the auxiliary calibration data. All individual readouts in the input scan data are separated and then corrected for dark signal by subtraction of the selected dark signal correction.

For band 1a measurements, where the integration time is significantly longer than for other channels/ bands, an additional correction, characterised by one value for the complete band, is needed for those measurements taken in the SAA (see Section 5.7.8). The correction is calculated using the blind pixels at the beginning of band 1a. The first m (~50) pixels of the channel 1a measurement are sorted with respect to signal intensity. The intensity of the k-th (~5) sorted pixel provides the additional correction which is then subtracted from the whole band. The additional correction in the SAA is written to the level 1a product as an appended parameter.

The shot and read-out noise on the corrected measurements is calculated from the raw binary units after subtraction of the dark signal. For band 1a in the SAA this is done before subtraction of the additional correction term. The flag F_{SAA} which is set to 1 for a pre-defined area during level 0 to 1a processing (see AG.8) is updated depending on the SAA intensity check using band 1a blind pixel data, and written to the PCD_BASIC record for level 1b data only.

5.7.11.3 Variables

5.7.11.3.1 *Local variables*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
k	Detector pixel index	i	-	t	-	
b	Bit string index for *FSAA*	i	-	t	-	*0 ..31*
S_1^{sort}	Sorted dark signal corrected detector pixel readouts	d[SAA_{sort}]	BU	t		

5.7.11.3.2 *Input from initialisation dataset*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
δ_{dt}	Dark signal detector temperature tolerance	d	K	i	A2.0.1, A3.0.1	
SAA_{pix}	Band 1a detector pixel number for SAA correction estimate	i	-	i	A2.0.1, A3.0.1	
SAA_{sort}	Number of band 1a detector pixels to be sorted for SAA correction estimate	i	-	i	A2.0.1, A3.0.1	
SAA_{thresh}	Threshold signal for SAA detection	d	BU/s	i	A2.0.1, A3.0.1	
SAA_{1a}	Flag indicating whether to apply the additional dark signal correction to band 1a measurements in the SAA	bool	-	i	A2.0.1, A3.0.1	1 = correct 0 = do not correct
pe	Number of photo-electrons per BU for each channel	i[B]	BU^{-1}	i	A2.0.1, A3.0.1	

5.7.11.3.3 *Input from in-flight calibration dataset or level 1a data stream*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
DS	Dark signal correction	d[D,B]	BU	i	A2.0.6, A3.0.4	**VIADR-1a-Dark** DARK_SIGNAL
σ_D	Readout noise on dark signal correction	d[D,B]	BU	i	A2.0.6, A3.0.4	**VIADR-1a-Dark** DARK_READOUT_NOISE
DS_{dt}	Mean detector temperature for which dark signal correction is valid	d[B]	K		A2.0.6, A3.0.4	

5.7.11.3.4 Input/output from other functions or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
dt	Detector temperature to be used for sorting of *dark* observation mode scans	d	-	i	A2.2, A3.0.4	**MDR-1a-***FPA_TEMP
IT	Integration time per band	d[B]	s	i	A2.2, A3.0.4	**MDR-1a-***INTEGRATION_TIMES
F_{SAA}	Flag indicating that scan is in SAA	bit-string [32]	-	i	A2.7, A3.0.4	**MDR-1a-***PCD_BASICF_SAA 1 = in SAA 0 = not in SAA
pmd_transfer	PMD transfer mode to be used for sorting of *dark* observation mode scans	enum	-	i	A2.3.1, A3.0.4	**MDR-1a-***PMD_TRANSFER
pmd_readout	PMD readout mode to be used for sorting of *dark* observation mode scans	enum	-	i	A2.3.1, A3.0.4	**MDR-1a-***PMD_READOUT

5.7.11.3.5 Input from level 0 or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
S^{BU}	Signal readout to be corrected for dark signal	d[D,B]	BU	i	A2.0.7, A3.0.4	**MDR-1a-***BAND_*

5.7.11.3.6 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
S_D^{BU}	Signal readout corrected for dark signal	d[D,B]	BU	o	various	
E_D^{BU}	Absolute error in dark corrected signal	d[D,B]	BU	o	various	

5.7.11.4 Algorithm

5.7.11.4.1 Select Dark Signal Correction (AG.11.1)

The appropriate dark signal correction is selected on the basis of detector temperature (*dt)*, integration time *(IT)*, PMD transfer mode *(pmd_transfer)* and PMD readout mode *(pmd_readout)*.
Note that in the case of signals co-added on-board the *actual* integration time (not the *effective* integration time after co-adding) is used. For a given combination of integration time PMD transfer mode and PMD readout mode, go back in time until you find a dark signal correction where the average detector temperature DS_{dt} is not more than δ_{dt} different from the current detector temperature *dt*. If this dataset is no longer within the valid time range as described in Section 5.1.2, the processing shall continue using these data, a report shall be raised via the MCS and the products shall be flagged as degraded using the fields DEGRADED_PROC_MDR and PCD_BASIC F_OLD_CAL_DATA in the level 1a and 1b products as specified in [AD5].

5.7.11.4.2 Subtract Dark Signal (AG.11.2)

The dark signal correction is applied for $i = 0 ... D_j - 1$, $j = 1...B$ as:

$$S_{D,ij}^{BU} = S_{ij}^{BU} - DS_{ij}$$

Equation 367

5.7.11.4.3 Apply Additional Correction For Band 1a In The SAA (AG.11.3)

For band 1a readouts for which $F_{SAA} = 1$ and $SAA_{1a} = 1$ the first SAA_{sort} dark signal corrected detector pixels are sorted on the basis of pixel intensity in ascending order to yield $S_{D,i1}^{sort}$. Calculate the normalised mean intensity of the first SAA_{sort} dark signal corrected detector pixels as follows:

$$\overline{S_1^{SAA}} = \sum_{i=0}^{SAA_{sort}-1} \frac{S_{D,i1}^{sort}}{SAA_{sort} \cdot IT_1}$$

Equation 368

Then if $\overline{S_1^{SAA}} > SAA_{thresh}$ then apply the additional correction for band 1a $S_{D,k1}^{sort}$ where $k = SAA_{pix}$ so that for $i = 0...D_1 - 1$:

$$S_{D,i1}^{BU} = S_{D,i1}^{BU} - S_{D,k1}^{sort}$$

Equation 369

5.7.11.4.4 Calculate Absolute Error on Corrected Measurement (AG.11.4)

- The absolute error in the corrected measurements, including a contribution for the readout noise on the dark signal correction, is this:

$$E_{D,ij}^{BU} = \sqrt{2 \cdot \sigma_{D,ij}^2 + \frac{S_{D,ij}}{e_j}} \qquad \text{Equation 370}$$

- If $F_{SAA} = 1$ $SAA_{1a} = 1$, and $\overline{S_1^{SAA}} > SAA_{thresh}$ then the absolute error in the band 1a corrected measurements, including an estimate of the error in the additional correction term SAA is given by:

$$E_{D,i1}^{BU} = \sqrt{2 \cdot \sigma_{D,i1}^2 + \frac{S_{D,i1}}{e_1} + (S^{sort}{}_{k1} - S^{sort}{}_{(k-1)1})^2} \qquad \text{Equation 371}$$

5.7.11.4.5 Update SAA Flag (AG.11.5)

The SAA flag is written out as a 32 bit string per scan. In AG.8, if $SAA_{1a} = 1$, $F_{SAA,b} = 1$ is initialised to *1* for $b = 0...31$ if the scan lies within a fixed geographical region covering the SAA.
Here the flag is updated on the basis of the band 1a readouts themselves.

Loop over all readouts k where $k = 0...R_{FPA} - 1$.

If $\overline{S_1^{SAA}} \le S_{thresh}$ then

if $IT_1 = 1.5s$ and $k > 0$ set $F_{SAA,b} = 0$ for $(k-1) \cdot 8 \le b < (k-1) \cdot 8 + 8$ else,

if $IT_1 = 6.0s$ set $F_{SAA,b} = 0$ for $0 \le b < 31$.

Otherwise $F_{SAA,b} = 1$ for $0 \le b < 31$.

End of Loop

The back-scan bit array is only updated in the case that all forward scan bit flags have been set to 0.

For $IT_1 = 1.5s$ and $k = 0$ and if $F_{SAA,b} = 0$ for all of $0 \le b < 23$, then set $F_{SAA,b} = 0$ for $24 \le b < 31$.

5.7.12 NORMALISE SIGNALS TO ONE SECOND INTEGRATION TIME (AG.12)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.12.1 Objectives

To normalise all signals previously corrected for Dark Signal to an effective Integration Time of one second.

5.7.12.2 Description

The signal detector readouts and their errors must at a minimum have been previously corrected for dark signal. Other calibration corrections may or may not have been applied as required. The detector signal readouts and their errors are normalised to an effective integration time of one second through division by the Integration Time specified in seconds. Note that in the case of signals co-added on-board the *actual* integration time (not the *effective* integration time after co-adding)

5.7.12.3 Variables

5.7.12.3.1 Input/output from other functions or level 1a data stream

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
S_D^{BU}	Detector signal readout corrected for dark signal	d[D,B]	BU	i	A2.9, A3.3	
E_D^{BU}	Error in detector signal readouts corrected for dark signal	d[D,B]	BU	i	A2.9, A3.3	
IT	Integration time for each band	d[B]	s	i	A2.2, A3.0.4	**MDR-1a-*** INTEGRATION_TIMES

5.7.12.3.2 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
S_D	Detector signal readouts corrected for dark signal and normalised to an integration time of one second	d[D,B]	BU/s	o	various	
E_D	Error in detector signal readouts corrected for dark signal and normalised to an integration time of one second	d[D,B]	BU/s	o	various	

5.7.12.4 Algorithm

For $i = 0...D_j - 1$, $j = 1...B$:

$$S_{D,ij} = \frac{S^{BU}_{D,ij}}{IT_j}$$ *Equation 372*

$$E_{D,ij} = \frac{E^{BU}_{D,ij}}{IT_j}$$ *Equation 373*

Note: For the PMD channels, the actual integration time depending on the readout mode and detector pixel block has to be used. See Appendix B.

5.7.13 APPLY PPG CORRECTION (AG.13)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.13.1 Objectives

To correct all measurements, excluding those from *dark* calibration mode for PPG.

5.7.13.2 Description

The PPG correction is applied only after the correction for dark signal (see Section 5.3.5) and normalisation to one-second integration time (see Section 5.3.6). All individual readouts in the input scan are separated. The PPG correction for each detector pixel of each channel is applied by dividing each detector pixel readout by the corresponding pixel of the PPG correction. The error in PPG adds to the noise which has been calculated in the application of dark signal. It is based on an estimate of the error in the pixel-to-pixel gain correction provided as part of the initialisation data. Note that PPG correction can only be applied to PMD data in raw transfer mode. If this is not the case PPG correction is not applied to the PMD data.

5.7.13.3 Variables

5.7.13.3.1 Local Variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
k	Detector pixel index counter for PPG correction	i	-	t		

5.7.13.3.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
δ_{PPG}	PPG error estimate for each channel	d[B]	-	i	A2.0.1, A3.0.1	

5.7.13.3.3 Input from in-flight calibration dataset or level 1a data stream

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
PPG	Pixel to Pixel Gain correction	d[D,B]	-	i	A2.0.6, A3.0.4	**VIADR-1a-PPG** PPG

5.7.13.3.4 Input/output from other functions or level 1a data stream

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
pmd_transfer	PMD transfer mode	enum	-	i	A2.3.3, A3.0.4	**MDR-1a-*** PMD_TRANSFER
S_D	Signal readout corrected for dark signal and normalised to one-second integration time	d[D,B]	BU/s	i	A2.10, A3.4	
E_D	Error in detector signal readouts corrected for dark signal and normalised to an integration time of one second	d[D,B]	BU/s	i	A2.10, A3.4	

5.7.13.3.5 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
S_{DP}	Signal readout corrected for dark signal and PPG and normalised to one-second integration time	d[D,B]	BU/s	o	various	
E_{DP}	Absolute error in PPG corrected signal	d[D,B]	BU/s	o		

5.7.13.4 Algorithm

If *pmd_transfer* = raw (i.e. PMD data is transferred in raw mode) the PPG correction is applied to both main and PMD channels. Otherwise the PPG correction is applied to main channels only. Nothing is done for PMD channels.

5.7.13.4.1 Apply PPG Correction (AG.13.1)

For $i = 0...D_j - 1$, $j = 1...B$, apply the PPG correction as follows:

$$S_{DP,\,ij} = S_{D,\,ij} / PPG_{ij}$$

Equation 374

5.7.13.4.2 Calculate Absolute Error on Corrected Measurement (AG.13.2)

For $i = 0...D_j - 1$, $j = 1...B$, calculate the absolute error as follows:

$$E_{DP,\,ij} = \sqrt{{E_{D,\,ij}}^2 + (\delta_{PPG,\,j} \cdot S_{DP,\,ij})^2}$$

Equation 375

5.7.14 APPLY SPECTRAL CALIBRATION (AG.14)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.14.1 Objectives

Perform spectral calibration of main channel and/or PMD spectra, thereby converting detector pixel numbers into the corresponding wavelengths.

5.7.14.2 Description

This module assigns a wavelength to each detector pixel of the main channels and the PMD channels. This is in fact the only calibration step which is not applied to the measured signals.

The module uses the pre-calculated spectral calibration parameters *ajm* from modules Calculate Spectral Calibration Parameters for Main Channels (A2.13) and Calculate Spectral Calibration Parameters for PMD Channels (A2.14) which are the polynomial coefficients for the conversion from detector pixel numbers to wavelengths. Pre-disperser prism temperature is used to select the appropriate set of spectral calibration coefficients.

5.7.14.3 Variables

5.7.14.3.1 Indices

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
m	Polynomial coefficient index	i	-	t	-	0…Mj

5.7.14.3.2 Input from initialisation dataset or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{PMD}	Total number of PMD bands	w	-	i	A2.0.1, A3.0.1	
δ_{pdp}	Pre-disperser prism temperature tolerance	d	K	i	A2.0.1, A3.0.1	
M	Order of wavelength calibration polynomial per channel	i[B]	-	i	A2.0.1, A3.0.1	

5.7.14.3.3 Input from in-flight auxiliary calibration dataset or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
a	Polynomial coefficients for spectral calibration	d[B, max (M)]	nm	i	A2.0.6, A3.0.4	**VIADR-1a-Spec** POLY_COEFF_FPA See Equation 75.
λ_{PMD}	Full spectral calibration grid for PMDs	d[B,D]	nm	i/o	A2.0.6, A3.0.4/various	
SLS_{pdp}	Mean pre-disperser prism temperature for which spectral calibration is valid	d	K	i	A2.0.6, A3.0.4	

5.7.14.3.4 Input from level 0 data stream and level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
s	Pixel number defining the start of a PMD band	$i[N_{PMD}]$	-	i	A2.0.7, A3.0.4	
l	Length in pixels of a PMD band	$i[N_{PMD}]$	-		A2.0.7, A3.0.4	

5.7.14.3.5 Input/output from other functions or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
pdp	Pre-disperser prism temperature for selection of spectral calibration parameters	d	K	i	A2.2, A3.0.4	**MDR-1a-*** PDP_TEMP
pmd_transfer	PMD transfer mode	enum[N]	-		A2.3, A3.0.4	**MDR-1a-*** PMD_READOUT
j_{min}	First channel for which spectral calibration will be applied	i	- i		various	1…*B*
j_{max}	Last channel for which spectral calibration will be applied	i	-		various	1…*B*

i
i

5.7.14.3.6 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
λ	Wavelength	d[D,B]	nm	o	various	**MDR-1b-Earthshine**WAVELENGTH_*

5.7.14.4 Algorithm

- If *pmd_transfer* = *raw* (i.e. PMD data is transferred in raw mode) the following calculations are carried out for both main and PMD channels. If *pmd_transfer* = *band* + *mixed* or *pmd_transfer* = *band* + *raw* then the following calculations are carried out unchanged for main channel data only.
- Go back in time until you find spectral calibration parameters where the average detector temperature DS_{dt} is not more than δ_{dt} different from the current detector temperature *dt*. If this dataset is no longer within the valid time range as described in Section 5.1.2, the processing shall continue using these data, a report shall be raised via the MCS and the products shall be flagged as degraded using the fields DEGRADED_PROC_MDR and PCD_BASICF_OLD_CAL_DATA in the level 1a and 1b products as specified in [AD5].
- For all Main channel data the wavelength of detector pixel *i* in channel *j* (where $j = j_{min}\ldots j_{max}$) is given by the equation:

$$S_{DP,\,ij} = S_{D,\,ij}/PPG_{ij}$$

Equation 376

- where the a_{jm} are the spectral calibration parameters from modules Calculate Spectral Calibration Parameters for Main Channels (A2.13). For *pmd_transfer* = *raw* calculate Spectral Calibration Parameters for PMD Channels (A2.14) provides the PMD spectral data on the full wavelength grid λ_{PMD}.
- If *pmd_transfer* = *band* + *mixed* or *pmd_transfer* = *band* + *raw* then for those data packets where PMD data are in band mode calculate the central pixel for each PMD band for $k = 1 \ldots N_{PMD}$, $j = p$ and $j = s$ as follows:

$$i_k^{cent} = s_k + (l_k - 1)/2$$

Equation 377

Note that i_k^{cent} may be non-integer. Then calculate the wavelength associated with PMD band k as $\lambda_{\mathrm{PMD},\, i_k^{cent}}$.

- The indices j_{min} and j_{max} are used to restrict the calculations to the channels for which spectral calibration is actually needed (e.g., calibrate main channels only, calibrate PMD channels only).

5.7.15 APPLY ETALON CORRECTION (AG.15)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.15.1 Objectives

To correct all measurements, excluding those from *dark*, *LED* and *SLS* calibration modes for Etalon.

5.7.15.2 Description

The Etalon correction is applied only after the correction for dark signal (see Section 5.3.5), normalisation to one-second integration time (see Section 5.3.6) and PPG correction (see Section 5.3.7). All individual readouts are read from the scan. The Etalon correction must be interpolated from its own wavelength grid to that of the measurement to be corrected. This is done using Spline Interpolation (AX.3). The Etalon correction for each detector pixel of each channel is then applied by dividing each detector pixel readout by the corresponding pixel of the interpolated Etalon correction. Note that Etalon correction can only be applied to PMD data in raw transfer mode. If this is not the case, Etalon correction is not applied to the PMD data.

5.7.15.3 Variables

5.7.15.3.1 Local variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
k	Detector pixel index counter for Etalon correction	i	-	t	-	0…Mj

5.7.15.3.2 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
δ_{Eta}	Etalon error estimate for each channel	d[B]	-	i	A2.0.1, A3.0.1	

5.7.15.3.3 Input from in-flight calibration dataset or level 1a data stream

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
λ^{ETN}	Wavelength grid of etalon correction	d[D,B]	nm	-		**VIADR-1a-Etalon** LAMBDA_ETALON
ETN	Etalon correction	d[D,B]	-	i	A2.0.6, A3.0.4	**VIADR-1a-Etalon** ETALON

5.7.15.3.4 Input/output from other functions or level 1a data stream

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
pmd_transfer	PMD transfer mode	enum	-	i	A2.3, A3.0.4	**MDR-1a-*** PMD_TRANSFER
S_{DP}	Signal readout corrected for dark signal, normalised to one-second integration time, corrected for PPG and spectrally calibrated	d[D,B]	BU/s	i	A2.12, A3.5	
λ	Wavelength grid of measurement to be corrected	d[D,B]	nm	i	A2.15, A3.6	

5.7.15.3.5 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
S_{DPE}	Signal readout corrected for dark signal, normalised to one-second integration time, corrected for PPG and Etalon and spectrally calibrated	d[D,B]	BU/s	o	various	
E_{DPE}	Absolute error in Etalon-corrected signal	d[D,B]	BU/s	o	various	

5.7.15.4 Algorithm

If *pmd_transfer* = raw (i.e. PMD data is transferred in raw mode) the Etalon correction is applied to both main and PMD channels. Otherwise the Etalon correction is applied to main channels only. Nothing is done for PMD channels.

5.7.15.4.1 Perform Wavelength Interpolation of Etalon Correction (AG.15.1)

Interpolate the Etalon correction *ETN* from its own wavelength grid λ^{ETN} to that of the measurement to be corrected λ using Spline Interpolation (AX.3) yielding $ETN(\lambda_{ij})$.

5.7.15.4.2 Apply Etalon Correction (AG.15.2)

For $i = 0...D_j - 1$, $j = 1...B$ apply the Etalon correction as follows:

$$S_{DPE,\,ij} = S_{DP,\,ij} / ETN(\lambda_{ij})$$ *Equation 378*

5.7.15.4.3 Calculate Absolute Error on Corrected Measurement (AG.15.3)

$$E_{DPE,\,ij} = \sqrt{E_{DP,\,ij}^{\;2} + (\delta_{Eta,\,j} \cdot S_{DPE,\,ij})^2}$$ *Equation 379*

5.7.16 DETERMINE STRAYLIGHT CORRECTION (AG.16)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

Spline Interpolation (AX.3)

Data Granule

One Scan

5.7.16.1 Objectives

To generate a stray light correction on the basis of measured detector readout intensity and stray light characterisation parameters determined on-ground.

5.7.16.2 Description

Stray light refers to the component of measured intensity for any given detector pixel, which originates from a wavelength other than that associated with that detector pixel. Two types of stray light will be considered, uniform stray light and ghost stray light.

Uniform stray light originates in diffuse scatter inside the instrument and generates a slowly varying or nearly uniform stray light across a detector array. Ghost stray light originates in specular reflections from optical components within the instrument. It is essentially focused on the detector array. One channel may contain several ghosts. Each ghost in a channel is associated with a parent detector pixel location. The ghost stray light correction for each detector pixel is a summation of scaled intensities from all contributing parent locations in the channel. Each ghost location is specified in the calibration Key Data as a polynomial function of parent pixel for each channel. The intensity of each ghost is specified as a polynomial function of parent pixel, subsequently scaled by the parent pixel intensity.

5.7.16.3 Variables

5.7.16.3.1 Local variables

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
k	Ghost index counter	i	-	t	-	
n	Readout index counter	i	-	t	-	
g	Ghost detector pixel grid	d[N^G,D,B]	-	t	-	See table that follows for an explanation for N^G
S^{mir}	Mirrored spectra from ghost stray light, given on ghost detector pixel grid	d[N^G,D,B]	BU/s	t	-	
$\hat{S}^{mir}$	Mirrored spectra from ghost stray light, interpolated back to detector pixel grid	d[N^G,D,B]	BU/s	t	-	
$\overline{S_{DPE}}$	Signals co-added to an effective integration time of band 1a	d[D,B]	BU/s	t	-	
S_{US}	Uniform stray light correction	d[B]	BU/s	t	-	
S_{GS}	Ghost stray light correction	d[D,B]	BU/s	t	-	

5.7.16.3.2 Input from key dataset

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
F	Uniform stray light fraction per channel (intra-channel only)	d[B]	-	i		
N^G	Number of stray light ghosts for each channel (intra-channel only)	i[B]	-	i	A2.0.4, A3.0.3	N^G without subscript as used for array dimensions in column "Type" means the maximum number of stray light ghosts (the maximum element of N^G)
l	Polynomial coefficients describing the intensity of stray light ghosts	d[3,N^G,B]	-		A2.0.4, A3.0.3	
p	Polynomial coefficients describing the location of stray light ghosts	d[3,N^G,B]	-i	i	A2.0.4, A3.0.3	

5.7.16.3.3 Input/output from other functions or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
λ	Wavelength grid of measurement to be corrected	d[D,B]	nm	i	A2.15, A3.6	
S_{DPE}	Signal readout corrected for dark signal, normalised to one-second integration time, corrected for PPG and Etalon and spectrally calibrated	d[D,B]	BU/s	i	A2.17, A3.7	

5.7.16.3.4 Input from level 0 data stream or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
IT	Integration time for each band	d[B]	s	i	A2.2, A3.0.4	**MDR-1a-*** INTEGRATION_TIMES

5.7.16.3.5 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
S_{Stray}	Stray light correction for each channel	d[D,B]	BU/s	o	A2.19, A3.9	

5.7.16.4 Algorithm

5.7.16.4.1 Sum Readouts to Effective Integration Time of Band 1a (AG.16.1)

For the calculation of stray light in band 1a, with a nominal integration time of 6s, significantly longer than for the remaining bands due to the low light levels in the UV, it is necessary to sum the readouts from the remaining bands to an effective integration time equivalent to that of band 1a.

For $i = 0...D_j - 1$ and $j = 1...B$ then

$$N_j = \frac{IT_{1a}}{IT_j}$$ *Equation 380*

and

$$\overline{S_{DPE,ij}} = \frac{1}{N_j} \cdot \sum_{n=1}^{N_j} S^n_{DPE,ij}$$ *Equation 381*

where *n* indicates the readout number.

In the calculation of stray light for band 1a it is assumed that for those contributions from the remaining bands the summed readouts corresponding to an effective integration time equivalent to that of band 1a will be used. For the calculation of stray light in the remaining bands the contribution of stray light from band 1a is expected to be insignificant and therefore the longer integration time of band 1a does not need to be taken into account. For the remaining calculations it is not necessary to distinguish main channel bands.

5.7.16.4.2 Determine Uniform Stray light (AG.16.2)

Uniform stray light is calculated, taking into account only intra-channel stray light, for all channels $j = 1...B$ as:

$$S_{US,j} = \frac{F_j}{D_j} \cdot \sum_{i=0}^{D_j - 1} S_{DPE,ij}$$ *Equation 382*

5.7.16.4.3 Determine Ghost Straylight (AG.16.3)

For all channels $j = 1...B$, all ghosts within a channel $k = 1...N_j^G$, and all parent detector pixels $i = 0...D_j - 1$, calculate the mirrored intra-channel ghost spectra as:

$$S^{\text{mir}}(g_{kij}) = S_{\text{DPE},\, ij} \cdot (I_{0kj} + I_{1kj}i + I_{2kj}i^2)$$ *Equation 383*

where the *ghost* detector pixel position is given by the following:

$$g_{kij} = p_{0kj} + p_{1kj}i + p_{2kj}i^2$$ *Equation 384*

For all channels $j = 1...B$, and all ghosts within a channel $k = 1...N_j^G$, and all ghosts within a channel , interpolate the mirrored ghost spectra $s^{\text{mir}}(g_{kij})$ from the ghost detector pixel grid g_{kij} onto the pixel grid of the measurement $i = 0...D_j - 1$ using Spline Interpolation (AX.3), yielding $\hat{S}_{kij}^{\text{mir}}$.

Calculate the ghost stray light for $i = 0...D_j - 1$ and $j = 1...B$ as follows:

.

$$S_{GS,\, ij} = \sum_{k=1}^{N_j^G} \hat{S}_{kij}^{\text{mir}}$$ *Equation 385*

5.7.16.4.4 Calculate Total Stray light (AG.16.4)

The total stray light correction is calculated for $i = 0...Dj - 1$ and $j = 1...B$ as:

$$S_{stray,\, ij} = S_{US,\, j} + S_{GS,\, ij}$$

5.7.17 APPLY STRAYLIGHT CORRECTION (AG.17)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

None

Data Granule

One Scan

5.7.17.1 Objectives

To correct all measurements taken in *Sun observation* mode and *Earth* mode for stray light.

5.7.17.2 Description

The measured signal is corrected for stray light by subtraction of the stray light correction. It is assumed that the measured signal has previously been corrected for dark signal, normalised to one-second integration time, corrected for PPG, Etalon and in addition has been spectrally calibrated.

5.7.17.3 Variables

5.7.17.3.1 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
δ_{Stray}	Stray light error estimate for each channel	d[B]	-	i	A2.0.1, A3.0.1	

5.7.17.3.2 Input from other functions

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
S_{DPE}	Signal readout corrected for dark signal, normalised to one-second integration time, corrected for PPG and Etalon and spectrally-calibrated	d[D,B]	BU/s	i	A2.17, A3.7	
E_{DPE}	Absolute error in Etalon-corrected signal	d[D	BU/s	i	A2.17, A3.7	
S_{Stray}	Stray light correction	d[D	BU/s	i	A2.17, A3.7	

5.7.17.3.3 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
S_{DPES}	Detector readout signal corrected for stray light	d[D,B]	BU/s	o	various	
E_{DPES}	Absolute error in corrected signal	d[D,B]	BU/s	o	various	

5.7.17.4 Algorithm

5.7.17.4.1 Apply Stray light Correction (AG.17.1)

The stray light correction is applied for $i = 0...Dj - 1$ and $j = 1...B$ as:

$$S_{DPES,\,ij} = S_{DPE,\,ij} - S_{stray,\,ij}$$

Equation 386

5.7.17.4.2 Calculate Absolute Error on Corrected Measurement (AG.17.2)

For $i = 0...Dj - 1$ and $j = 1...B$ calculate the following:

$$E_{DPES,\,ij} = \sqrt{E_{DEP,\,ij}^{\;2} + (\delta_{Stray} \cdot S_{DPES,\,ij})^2}$$

Equation 387

5.7.18 APPLY IRRADIANCE RESPONSE (AG.18)

Uses Generic Sub-Function:

Calculate MMEs for PMD Data in Band Transfer Mode (AG.3)

Uses Auxiliary Sub-Functions:

Linear Interpolation (AX.2)

Data Granule

One Scan, with access to the previous scan

5.7.18.1 Objectives

To correct *Sun* observation mode measurements for the irradiance response of the instrument and to calculate both the total absolute error and the contribution due to random noise.

5.7.18.2 Description

GOME-2 measures solar spectra during *Sun* observation mode (Section 2.3.3). An on-board diffuser is placed in the light path during *Sun* observation mode to scatter the collimated solar irradiance into a diffuse radiance beam. During *Sun* observation mode, the Sun moves through the FOV of the diffuser in elevation direction. The solar azimuth angle does not change significantly during the time interval of Sun observation, but depends on season. The MMEs describing the irradiance response of the instrument (Section 5.2.3) are calculated for the wavelength calibration of the SMR spectrum applicable at the time of the pre-processing of the MMEs. Furthermore they are pre-calculated for a fine grid of solar elevation and azimuth angles. Before correcting for the irradiance response of the instrument, the MMEs are further interpolated to the solar elevation and azimuth angle of the measurement, and the current wavelength grid of the *Sun* observation mode measurements. In the case of PMD data transferred in *band + raw* or *band + mixed* transfer modes, MMEs appropriate to PMD band data as calculated in Section 5.7.18.4 should be selected. Also calculated are the total absolute error in the corrected spectrum and the contribution due to random noise.

5.7.18.3 Variables

5.7.18.3.1 Local variables

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
e_{meas}	Solar elevation angle of the measurement (Satellite Relative Actual Reference CS)	d	degree	t	-	
θ_{meas}	Solar zenith angle provided on the fixed integration time grid (Satellite Relative Actual Reference CS)	d	degree	t	-	
φ_{meas}	Solar azimuth angle provided on the fixed integration time grid (Satellite Relative Actual Reference CS)	d	degree	t	-	

5.7.18.3.2 Input from initialisation dataset or level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
N_{ef}	Number of solar elevation angles for which the fine elevation angle grid is specified	w	-	i	A2.0.1, A3.0.4	
$N_{\varphi f}$	Number of solar azimuth angles for which the fine azimuth angle grid is specified	w	-	i	A2.0.1, A3.0.4	
e_f	Solar elevation angles which define the fine elevation angle grid (Satellite Relative Actual Reference CS)	$d[N_{ef}]$	degree	i	A2.0.1, A3.0.4	
φ_f	Solar azimuth angles which define the fine azimuth angle grid (Satellite Relative Actual Reference CS)	$d[N_{\varphi f}]$	degree	i	A2.0.1, A3.0.4	
NPMD	Total number of PMD bands	w	-	i	A2.0.1, A3.0.1	
pe	Number of photo-electrons per BU for each channel	i[B]	BU^{-1}	i	A2.0.1, A3.0.1	

5.7.18.3.3 Input from in-flight calibration dataset and level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
σ_D	Readout noise	d[D,B]	BU	i	A2.0.6, A3.0.4	**VIADR-1a-Dark** DARK_READOUT_NOISE

5.7.18.3.4 Input/output from other functions and level 1a data stream

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
$M^{1,irrad}$	Müller matrix element describing the irradiance response of the instrument to unpolarised light	d[D,B, N_{ef}, $N_{\varphi f}$]	$BU.s^{-1}/(photons/(s.cm^2.nm))$	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_IRRAD_RESP
$\varepsilon\_M^{1,irrad}$	Relative error in the Müller matrix element describing the irradiance response of the instrument to unpolarised light	d[D,B]	-	i	A2.1, A3.0.4	**GIADR-1a-MME** MME_ERR_IRRAD_RESP
IT	Integration time per band	i[B]	s	i	A2.2, A3.0.4	**MDR-1a-*** INTEGRATION_TIMES
pmd_transfer	PMD transfer mode	enum	-	i	A2.3, A3.0.4	**MDR-1a-*** PMD_TRANSFER
θ_{Sun}	Solar zenith angle provided on the fixed integration time grid (Satellite Relative Actual Reference CS)	d[35,3]	degree	i	A2.6, A3.0.4	**MDR-1a-*** GEO_BASICSOLAR_ZENITH_ANGLE
φ_{Sun}	Solar azimuth angle provided on the fixed integration time grid (Satellite Relative Actual Reference CS)	d[35,3]	degree	i	A2.6, A3.0.4	**MDR-1a-*** GEO_BASICSOLAR_AZIMUTH_ANGLE
λ^{sun}	Wavelength grid of the measured solar spectrum	d[D,B]	nm	i	AG.14	
$Sun^{BU/s}$	Solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light normalised to an effective integration time of one second.	d[D,B]	BU/s	i	AG.17	

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
E_{DPES}	Absolute error in solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light normalised to an effective integration time of one second.	d[D,B]	BU/s	i	AG.17	

5.7.18.3.5 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
Sun	Solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light and the irradiance response of the instrument.	d[D,B]	photons/(s.cm^2.nm)	o	A2.20, A3.17.1	**MDR-1b-Sun** BAND_*RAD
ESun	Absolute error in solar measurements taken in *Sun* observation mode corrected for dark signal, PPG, Etalon and stray light and the irradiance response of the instrument.	d[D,B]	photons/(s.cm^2.nm)	o	A2.20, A3.17.1	**MDR-1b-Sun** BAND_*ERR_RAD
Erand	Random noise contribution to the total absolute error	d[D,B]	photons/(s.cm^2.nm)	o	A2.20	

5.7.18.4 Algorithm

5.7.18.4.1 Calculate MMEs For PMD Data In Band Transfer Mode (AG.18.1)

In the case of PMD data transferred in *band + mixed* or *band + raw* transfer modes MMEs and their errors which are band averaged should be used. In this case it is necessary to calculate the MMEs and their ratios as the mean value over the PMD bandwidth. Mean errors are also calculated as appropriate. This is done using Calculate MMEs for PMD Data in Band Transfer Mode (AG.3). These calculations need only be repeated if the PMD band definition is changed.

In the subsequent algorithm descriptions no distinction is made in notation between standard MMEs or those which have been band-averaged for PMD channels as described above. If PMD data is transferred in *band + mixed* or *band + raw* transfer modes the index i for PMD channels $j = 5$ or $j = 6$ will refer to PMD bands and will lie in the range $i = 1...N_{PMD}$. In all other cases it will refer to detector pixel number.

5.7.18.4.2 Interpolate MME Describing Irradiance Response (AG.18.2)

- Calculate the appropriate solar zenith angle θ_{meas} and solar azimuth angle φ_{meas} from the set of basic geolocation parameters calculated in Calculate Geolocation for Fixed Grid (A2.6) and provided in the level 1a product, θ_{Sun} and φ_{Sun} . These basic geolocation parameters are provided on a fixed 187.5ms integration time grid, see Section 5.2.8. For each readout the angles from the previous 187.5 ms period should be selected, i.e., angle n–1 corresponds to readout n. This is similar to the selection of angles in Apply Polarisation Correction (A3.10), see the ***Note*** in Section 5.3.12.4. If no previous readout is available, the output parameters for the current readout are set to “undefined” and the flag for degraded MDR quality due to a processing degradation (DEGRADED_PROC_MDR) is raised. (This is not applicable if this module is called from Calculate SMR (A2.20) as in this case a subset of readouts has been pre-selected, so that a previous readout will always be available.) For PMD readouts in raw transfer mode the packet contains the last of the 16 readouts in the 375 ms, therefore the corresponding scanner angles are 4, 8, ... , 16. See also Figure 23.
- Convert the solar zenith θ_{meas} to solar elevation e_{meas} using Equation 403 in Appendix C.
- Interpolate the MME describing the irradiance response of the instrument from the fine azimuth and elevation angle grids φ_f and e_f to the elevation and azimuth angles of the measurement φ_{meas} and e_{meas} using Linear Interpolation (AX.2).
- Interpolate the MME describing the irradiance response of the instrument and its relative error from the fixed wavelength grid of the MMEs, λ^{MME}, to the wavelength grid of the measurement, using Spline Interpolation (AX.3). For spectral points of λ_{sun} outside λ^{MME} set the irradiance response of the instrument and its relative error equal to the first (or last) valid value on the original MME wavelength grid.

5.7.18.4.3 Correct for Irradiance Response (AG.18.3)

- The description below refers to main channels and PMD blocks CDE. For PMD block B set *Sun*, E_{Sun} and E_{rand}, and to be “undefined”.

- Correct for the irradiance response of the instrument, for $i = 0...D_j - 1$ and $j = 1...B$ as:

$$Sun = Sun^{BU/s} / (M^{1,irrad}_{e_{meas}, \varphi_{meas}}(\lambda^{sun}_{ij}))$$

Equation 388

5.7.18.4.4 Calculate Absolute Error (AG.18.4)

- Calculate the absolute error in the corrected spectrum, for $i = 0...D_J - 1$ and $j = 1...B$ as:

$$E_{Sun} = \frac{1}{M^{1,irrad}_{e_{meas}, \varphi_{meas}}(\lambda^{sun}_{ij})} \cdot \sqrt{E^2_{DPES} + (\varepsilon\_M^{1,irrad}(\lambda^{sun}_{ij}) \cdot Sun^{BU/s}_{ij})^2}$$

Equation 389

5.7.18.4.5 Calculate the Random Noise Contribution (AG.18.5)

Calculate the random noise contribution to the total error and correct for the irradiance response of the instrument, for $i = 0...D_J - 1$ and $j = 1...B$ as:

$$E_{rand} = \frac{1}{M^{1,irrad}_{e_{meas}, \varphi_{meas}}(\lambda^{sun}_{ij}) \cdot IT_j} \cdot \sqrt{\sigma^2_{D,ij} + (Sun^{BU/s}_{ij} \cdot IT_j)/e_j}$$

Equation 390

5.7.19 CORRECT DOPPLER SHIFT (AG.19)

Uses Generic Sub-Function:

Calculate MMEs for PMD Data in Band Transfer Mode (AG.3)

Uses Auxiliary Sub-Functions:

Linear Interpolation (AX.2)

Data Granule

FPA/PMD wavelength array.

5.7.19.1 Objectives

To correct the Doppler shift on the measured solar spectra due to the motion of the satellite.

5.7.19.2 Description

This module corrects the Doppler shift on measured solar spectra using the relative speed of satellite and sun. The solar spectrum with the corrected wavelength axis is the one GOME-2 would have observed if the satellite had not moved relative to the sun. Doppler correction of the solar spectra aligns the spectral features (in particular, the Fraunhofer lines) of solar and earthshine spectra which is an important prerequisite for rationing them. In the level 1a processor, this algorithm is applied on the wavelength grid of the SMR spectrum. In the level 1b processor, it is applied on the wavelength grid of individual spectra in the solar measurements mode.

Note: For Earthshine spectra, the velocity component along the line of sight is close to zero, i.e. the Doppler shift of the Earthshine spectra is negligible.

5.7.19.3 Variables

5.7.19.3.1 Input from initialisation dataset

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
c	Speed of light	d	m/s	i	A3.0.1	

5.7.19.3.2 Input from other functions

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
λ	Wavelength of solar spectrum not corrected for Doppler shift	d[D,B]	nm	i	A3.6	
$v_{Sat\text{-}Sun}$	Relative speed of satellite and sun (negative if satellite is moving towards the sun)	d	m/s	i	A2.20.4 or A3.0.4	**.MDR-1*SUN** GEO_SUNVEL_SAT_SUN In the case of the SMR, this is the mean relative speed.

5.7.19.3.3 Output

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
λ^{corr}	Wavelength of solar spectrum corrected for Doppler shift	d[D,B]	nm	o	A3.17.2	**MDR-1b-Sun** WAVELENGTH_*

5.7.19.4 Algorithm

Correct the wavelengths for the Doppler shift of the solar spectra using the following:

$$\lambda_{ij}^{corr} = \lambda_{ij}\left(1 - \frac{v_{\text{Sat-Sun}}}{c}\right) \qquad (i = 0\ldots D_j - 1, j = 1\ldots B)$$

Equation 391

The Doppler shift causes the spectral features in the observed solar spectrum to be blue-shifted because the satellite is moving towards the sun for GOME-2 solar calibrations. The correction shifts the wavelengths back to the red: As $v_{\text{Sat-Sun}}$ is negative, the corrected wavelengths will be larger than the uncorrected ones.

5.7.20 CALCULATE CENTRE COORDINATES (AG.20)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

Linear Interpolation (AX.2)

Data Granule

Two points on earth’s surface given by their latitude and longitude.

5.7.20.1 Objectives

To calculate geodetic latitude and geocentric longitude of the point at the centre of the geodesic line between two points specified by their geodetic latitude and geocentric longitude.

5.7.20.2 Description

Given two points on earth's surface described by their geodetic latitude and geocentric longitude, this module calculates the coordinates of the point at the centre of the geodesic line (great circle) between these two points. The module will be used when centre coordinates of a ground pixel have to be calculated from its corner coordinates. In this case, coordinates of two corner points on either side of a diagonal have to be provided on input.

The centre point is calculated internally in cartesian coordinates, so there are two coordinate system transformations needed. The exact algorithm depends on the functionality of the PGE services related to geolocation. For the purpose of this description it is assumed that there is a routine for converting geodetic into cartesian coordinates, called `ml_geo_car`, and a routine transforming cartesian to geodetic coordinates, called `ml_car_geo`.

5.7.20.3 Variables

5.7.20.3.1 Index

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
i	Cartesian coordinate	i	-	t	-	1...3
k	Index denoting point on earth's surface	i	-	t	-	1...2

5.7.20.3.2 Input/output from other functions

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
lon_1	Geocentric longitude of point 1 (earth-fixed CS)	d	degree	i		
lat_1	Geodetic latitude of point 1 (earth-fixed CS)	d	degree	i		
lon_2	Geocentric longitude of point 2 (earth-fixed CS)	d	degree	i		
lat_2	Geodetic latitude of point 2 (earth-fixed CS)	d	degree	i		

5.7.20.3.3 Local Variables

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
r_1	Cartesian position vector of point 1 (earth-fixed CS)	d[3]	m	t		
r_2	Cartesian position vector of point 2 (earth-fixed CS)	d[3]	m	t		
r_{Centre}	Cartesian position vector of centre point (earth-fixed CS)	d[3]	m	t		
s	Scaling factor	d	-	t		

5.7.20.3.4 Output

Symbol	Descriptive Name	Type	Units	I/O	Source	Remarks
lon_{Centre}	Geocentric longitude of centre point (earth-fixed CS)	d	degree	o		–180…+180
lat_{Centre}	Geodetic latitude of centre point (earth-fixed CS)	d	degree	o		–90…+90

5.7.20.4 Algorithm

Convert coordinates of the input points from longitude/latitude lon_k, lat_k, to cartesian coordinates r_k (k = 1, 2) using routine `ml_geo_car`, where geodetic altitude and all rates are set to zero on input.

Calculate cartesian coordinates of the centre point as follows:

$$r_{\text{Centre},\, i} = s(r_{1i} + r_{2i}) \qquad (i = 1, 2, 3)$$ *Equation 392*

where

$$s = \frac{1}{\sqrt{2\left(1 + \dfrac{r_1 \bullet r_2}{|r_1||r_2|}\right)}}$$ *Equation 393*

$$r_1 \bullet r_2 = \sum_i (r_{1i} r_{2i})$$ *Equation 394*

$$|r_k| = \sqrt{\sum_i r_{ki}^2} \qquad (k = 1, 2)$$ *Equation 395*

Convert coordinates of the centre point back from cartesian coordinates r_{Centre} to longitude/latitude lon_{Centre}, lat_{Centre} using routine `ml_car_geo`, where the cartesian velocity vector is set to zero on input. Convert lon_{Centre} to the ISO 6709 representation using equation (404) if needed.

5.8 AUXILIARY PROCESSING SUB-FUNCTIONS

5.8.1 Calculate Mean, Standard Deviation And Mean Error Of Readouts (AX.1)

Uses Generic Sub-Function:

None

Uses Auxiliary Sub-Functions:

Linear Interpolation (AX.2)

Data Granule

Many scans from one measurement mode period.

5.8.1.1 Objectives

To generate a mean readout value, standard deviation, and error in the mean from a number of input detector array readouts and their associated absolute error and noise values. A combined saturation and hot pixel mask is applied to each detector readout before calculation begins.

5.8.1.2 Description

This sub-function accepts a number of detector array readouts and generates a mean readout value for each detector pixel from each band. The associated standard deviation and error in the mean value are also calculated. The calculation of the error in the mean value takes account of the fact that the contribution of random noise sources is reduced according to the number of spectra being averaged. A combined saturation and hot pixel mask previously calculated in Determine PCDs from Raw Intensity (A2.4), is applied to all detector readouts. Any detector pixels flagged hot or any bands flagged as saturated are excluded from the calculation of the mean, standard deviation and mean noise.

5.8.1.2.1 Local variables

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
k	Readout index number	i	-	t	-	
N_{mask}	Number of readouts remaining after saturated and hot pixel masking per detector pixel and band	i[D,B]	-	t	-	
□E_{tot}□	Mean total error in signal readout values	d[D,B]	per input	t	-	
□E_{rand}□	Mean random error in signal readout values	d[D,B]	per input	t	-	
pixmask	Combined saturated and hot pixel mask	i[D,B,N]	-	t	-	1 = normal pixel 0 = hot or saturated pixel

5.8.1.2.2 *Input/output from other functions*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
N	Total number of detector pixel readouts to be averaged.	i[B]	-	i	various	
S	Signal readout values	d[D,B,N]	per input	i	various	
E_{tot}	Total error in signal readout values	d[D,B,N]	per input	i	various	*optional*
E_{rand}	Random noise contribution	d[D,B]	per input	i	-	*optional*
hotpix	Hot pixel mask	b[D,B,N]	-	i	A2.4	1 = normal 0 = hot
satpix	Saturation mask	b[B,N]	-	i	A2.4	1 = normal 0 = hot

5.8.1.2.3 *Output*

Symbol	*Descriptive Name*	*Type*	*Units*	*I/O*	*Source*	*Remarks*
□*S* □	Mean signal readout	d[D,B]	per input	o	various	
σ	Standard deviation of signal readout values	d[D,B]	per input	o	various	*only calculated if required*
□*E*□	Error in mean signal readout	d[D,B]	per input	o	various	*only calculated if required*
missing	Mask indicating missing mean values					1 = missing 0 = not missing

5.8.1.3 Algorithm

For $i = 0...D_j - 1$ and $j = 1...B$ and $k = 1...R$ then $pixmask_{ijk} = hotpix_{ijk} \times satpix_{jk}$. For PMD block C data, in *nominal* or *sun* readout mode, additionally set *pixmask* to be zero for readouts $k = 1, 3, 5,....$

The mean signal value for each detector pixel and band is calculated for $i = 0...D_j - 1$ and for $j = 1...B$ as follows:

$$\langle S_{ij} \rangle = \frac{1}{N_{mask,\,ij}} \cdot \sum_{k=1}^{N} (S_{ijk} \cdot pixmask_{ijk}) \text{ where}$$

Equation 396

$$N_{mask,\,ij} = \sum_{k=1}^{N_j} pixmask_{ijk}$$

Equation 397

Assuming N_{mask} and *missing* have been initialised to zero for $i = 0...D_j - 1$ and $j = 1...B$ if:

$$N_{mask,\,ij} = 0 \text{ then } missing_{ij} = 1$$

Equation 398

The standard deviation in the sample is then calculated as follows:

$$\sigma_{ij} = \sqrt{\frac{1}{N_{mask,ij} - 1} \cdot \sum_{k=1}^{N_j} (S_{ijk} - \langle S_{ij} \rangle)^2 \cdot pixmask_{ijk}}$$
$$= \sqrt{\frac{1}{(N_{mask,ij} - 1)} \left[\left(\sum_{k=1}^{N_j} (S_{ijk} \cdot pixmask_{ijk}) \right)^2 - N_{mask,ij} \cdot \langle S_{ij} \rangle^2 \right]}$$

Equation 399

In the case that the error and noise on the individual detector readouts are supplied as input then if:

$$\langle E_{tot} \rangle_{ij} = \frac{1}{N_{mask,ij}} \cdot \sum_{k=1}^{N_j} (E_{tot,ijk} \cdot pixmask_{ijk})$$

Equation 400

and

$$\langle E_{rand} \rangle_{ij} = \frac{1}{N_{mask,ij}} \cdot \sum_{k=1}^{N_j} (E_{rand,ijk} \cdot pixmask_{ijk})$$

Equation 401

the error in the mean signal is calculated as follows:

$$\langle E \rangle_{ij} = \sqrt{\langle E_{tot} \rangle_{ij}^2 - \left(\langle E_{rand} \rangle_{ij}^2 \cdot \left(\frac{N_{mask} - 1}{N_{mask}} \right) \right)}$$

Equation 402

If the error and random noise on the individual detector readouts are not supplied as input then nothing is done.

The following points should be noted. For the calculation of the mean, standard deviation and noise in the mean signal it is not necessary to retain all data points in memory. It is sufficient to keep a cumulative mean of the signal readouts, the square of the signal readouts, and the noise on the signal readouts.

5.8.2 LINEAR INTERPOLATION (AX.2)

Linear interpolation should be carried out using a standard algorithm such as that described in [RD10]. See Equations 3.3.1 and 3.3.2 on page 107 of this document.

5.8.3 SPLINE INTERPOLATION (AX.3)

Spline Interpolation should be carried out using a standard algorithm such as that described in Section 3.3 Cubic Spline Interpolation in document [RD10].

5.8.4 AKIMA INTERPOLATION (AX.4)

The Akima interpolation method attempts to produce a curve through a set of data points in such a way that the resultant curve will appear smooth and natural and similar to that drawn manually. The method does not assume any functional form for the curve as a whole but the slope of the curve is determined locally and the interpolation between two successive points is represented by a polynomial of degree three, at most. The polynomial is determined from the coordinates of and the slopes at the two points. Since the slope of the curve must also be determined at the end points of the curve, estimation of two more points is necessary at each end point.

Akima Interpolation should be carried out by implementing the algorithm described in [RD6].

APPENDIX A: SUMMARY OF APPLICABLE CALIBRATION STEPS AND CONFIGURABLE OPTIONS

The table below provides a summary of all applicable calibration and processing steps for each observation mode. Those for which the application is user configurable are also indicated. This information is included in the level 1a and 1b products in the records **GIADR-1a-Steps** and **GIADR-1b-Steps** as specified in [AD4] and [AD5].

Legend:

Y	Always applied
PMD	Applied on PMD data only
(...)	Optional (user-selectable)
N	Never applied
N/A	Separation into observation modes not applicable

Algorithm step	*Reference*	*Observation mode*								
		Earth	Dark	Sun	WLS	SLS	SLS over diffuser	LED	Moon	Other
Level 0 to 1a Processing	**A2**									
Read Input Data	A2.0	N/A								
Preprocess Müller Matrix Elements	A2.1	N/A								
Convert Housekeeping Data	A2.2	Y	Y	Y	Y	Y	Y	Y	Y	Y
Determine Observation Mode and Viewing Angles	A2.3	Y	Y	Y	Y	Y	Y	Y	Y	Y
Determine PCDs from Raw Intensity	A2.4	Y	Y	Y	Y	Y	Y	Y	Y	N
Prepare PMD Data	A2.5	Y	Y	Y	Y	Y	Y	Y	Y	N
Calculate Geolocation for Fixed Grid	A2.6	Y	Y	Y	Y	Y	Y	Y	Y	Y
Determine PCDs from Geolocation	A2.7	Y	Y	Y	Y	Y	Y	Y	Y	Y
Calculate Dark Signal Correction	A2.8	N	Y	N	N	N	N	N	N	N
Apply Dark Signal Correction	A2.9	PMD	N	Y	Y	Y	N	Y	N	N
Normalise Signals to One Second Integration Time	A2.10	PMD	N	Y	Y	Y	N	Y	N	N
Calculate PPG	A2.11	N	N	N	(Y)	N	N	Y	N	N
Apply PPG Correction	A2.12	N	N	Y	(Y)	Y	N	N	N	N
Calculate Spectral Calibration Parameters for Main Channels	A2.13	N	N	N	N	Y	N	N	N	N
Calculate Spectral Calibration Parameters for PMD Channels	A2.14	N	N	N	N	Y	N	N	N	N
Apply Spectral Calibration Parameters	A2.15	PMD	N	Y	(Y)	N	N	N	N	N
Calculate Etalon Correction	A2.16	N	N	N	(Y)	N	N	N	N	N

Algorithm step	*Reference*	*Observation mode*								
		Earth	**Dark**	**Sun**	**WLS**	**SLS**	**SLS over diffuser**	**LED**	**Moon**	**Other**
Apply Etalon Correction	A2.17	N	N	(Y)	N	N	N	N	N	N
Determine Stray light Correction	A2.18	(PMD)	N	(Y)	N	N	N	N	N	N
Apply Stray light Correction	A2.19	(PMD)	N	(Y)	N	N	N	N	N	N
Calculate SMR	A2.20	N	N	Y	N	N	N	N	N	N
Determine Stokes Fractions	A2.21	(PMD)	N	N	N	N	N	N	N	N
Collect Global PCDs per Product	A2.22	N/A								
Write Level 0 and 1a Product	A2.23	N/A								
Level 1a to 1b Processing	A3									
Read Input Data	A3.0	N/A								
Prepare PMD Data	A3.1	Y	Y	Y	Y	Y	Y	Y	Y	N
Calculate Geolocation for Actual Integration Times	A3.2	Y	N	N	N	N	N	N	N	N
Apply Dark Signal Correction	A3.3	(Y)	(Y)	(Y)	(Y)	(Y)	(Y)	(Y)	(Y)	N
Normalise Signals to One Second Integration Time	A3.4	(Y)	(Y)	(Y)	(Y)	(Y)	(Y)	(Y)	(Y)	N
Apply PPG Correction	A3.5	(Y)	N	(Y)	(Y)	(Y)	(Y)	(Y)	(Y)	N
Apply Spectral Calibration Parameters	A3.6	(Y)	N	(Y)	(Y)	(Y)	(Y)	N	(Y)	N
Apply Etalon Correction	A3.7	(Y)	N	(Y)	(Y)	(Y)	(Y)	N	(Y)	N
Determine Stray light Correction	A3.8	(Y)	N	(Y)	N	N	N	N	(Y)	N
Apply Stray light Correction	A3.9	(Y)	N	(Y)	N	N	N	N	(Y)	N

Algorithm step	*Reference*	*Observation mode*								
		Earth	Dark	Sun	WLS	SLS	SLS over diffuser	LED	Moon	Other
Apply Polarisation Correction	A3.10	(Y)	N	N	N	N	N	N	N	N
Apply Radiance Response	A3.11	(Y)	N	N	N	N	N	N	(Y)	N
Apply Irradiance Response	A3.12	N	N	(Y)	N	N	N	N	N	N
Correct Doppler Shift	A3.13	N	N	(Y)	N	N	N	N	N	N
Reduce Spatial Aliasing	A3.14	(Y)	N	N	N	N	N	N	N	N
Calculate Fractional Cloud Cover and Cloud Top Pressure	A3.15	(Y)	N	N	N	N	N	N	N	N
Collect Global PCDs per Product	A3.16	N/A								
Write Level 1b Product	A3.17	N/A								

Algorithm step	*Reference*	*Observation mode*								
		Earth	**Dark**	**Sun**	**WLS**	**SLS**	**SLS over diffuser**	**LED**	**Moon**	**Other**
Generic processing sub-functions		Applicability to modes is not repeated here.								
Initialise Orbit Propagator	AG.1	N/A								
Calculate MMEs for PMD Data in Band Transfer Mode	AG.3									
Convert Housekeeping Data	AG.4									
Prepare PMD Data	AG.5									
Check for Saturated Pixels	AG.6	See Section 5.2.6 *Determine PCDs from raw intensity*.								
Check for Hot Pixels	AG.7	See Section 5.2.6 *Determine PCDs from raw intensity*.								
Check for SAA	AG.8	See Section 5.2.6 *Determine PCDs from raw intensity*.								
Check for Sunglint	AG.9	See Section 5.2.6 *Determine PCDs from raw intensity*.								
Check for Rainbow	AG.10	See Section 5.2.6 *Determine PCDs from raw intensity*.								
Apply Dark Signal Correction	AG.11									
Normalise Signals to One Second Integration Time	AG.12									
Apply PPG Correction	AG.13									
Apply Spectral Calibration	AG.14									
Apply Etalon Correction	AG.15									
Determine Stray light Correction	AG.16									
Apply Stray light Correction	AG.17									
Apply Irradiance Response	AG.18									

Algorithm step	*Reference*	*Observation mode*								
		Earth	**Dark**	**Sun**	**WLS**	**SLS**	**SLS over diffuser**	**LED**	**Moon**	**Other**
Correct Doppler Shift	AG.19									
Calculate Centre Coordinates	AG.20									
Auxiliary processing sub-functions										
Calculate Mean, Standard Deviation and Mean Error of Readouts	AX.1									
Linear Interpolation	AX.2									
Spline Interpolation	AX.3									
Akima Interpolation	AX.4									

APPENDIX B: PMD READOUT AND TRANSFER MODES

Each of the two PMD channels is divided into five blocks, labelled from A to E.

Block	*Pixel range*	*Pixel range for Length(B) = 23*	*Approximate wavelength [nm]*	*Notes*
A		0…744		data always discarded
B	768–Length(B)…767	745…767	288…299	short wavelength fields
C	768…768 + Length(B) – 1	768…790	299…312	
D	768 + Length(B)…990	791…990	312…790	nominal block
E	991…1023	991…1023	> 790	

Table 6: Definition of pixel blocks in PMDs.

The number of detector pixels in block B, Length(B), is one of the GOME-2 default setting parameters (see [AD9] and [AD10]). The current default value for Length(B) is 23, the largest possible value is 35. Note that Length(B) = Length(C), and Length(CDE) = 256. Only block D is guaranteed to have good data quality. The usefulness of the other blocks will depend on the level of stray light. Data from block A are never visible outside the instrument.

PMD readout modes and data transfer modes have to be distinguished. The **readout mode** determines the sequence in which the individual blocks are read, and thereby the integration time per block. The data **transfer mode** determines how the data are transmitted to ground. There are combinations of full spectral with reduced temporal (spatial) sampling, and full temporal (spatial) with reduced spectral sampling, the latter one being achieved by onboard co-adding of detector pixels into spectral bands. The current PMD readout and transfer modes are indicated in the science data packet by their numbers.

There are three readout modes, adapted to different illumination conditions. They are summarised in Table 7.

Readout Mode	**IT Block B [ms]**	**IT Block C [ms]**	**IT Blocks DE [ms]**
(0) nominal mode	6000	46.875	23.4375
(1) solar mode	46.875	46.875	23.4375
(2) calibration mode	≥ 93.75		

Table 7: PMD readout modes

Readout mode 0: **nominal readout mode**

This is the default for nadir scanning observations. Blocks DE are read every 23.4375 ms (16 times during a 375 ms period). Block C is read every 46.875 ms. The remaining blocks (AB) are reset once per scan, i.e., every 6 seconds, during a particular subset of the back scan. The number of the subset used for reset is programmable. It is one of the GOME-2 default settings defined in the DSM table. The fields for PMD integration time and integration time status in the Science Data Packet have no meaning for this readout mode.

Note: The "PMD reset cycle of flyback" in the DSM table is given in units of 93.75 ms. To convert to a data subset number, it has to be divided by four.

Readout mode 1: **solar readout mode**

This is the default for solar observations. It is the same as readout mode 0 (nominal) with the single exception that block B is read every 46.875 ms. The fields for PMD integration time and integration time status in the Science Data Packet have no meaning for this readout mode.

Readout mode 2: **calibration readout mode** (also called LED readout mode)
This mode is used for several calibration measurements, in particular SLS, WLS, and LED measurements. In this mode all 1024 detector pixels of the detector are read out subsequently with integration times of 93.75 ms or multiples thereof, as it is done for main channels 3 and 4. The actual integration time and integration time status is indicated in the Science Data Packet in the same way as it is done for the main channels.

There are also three data transfer modes:

Transfer mode 1: **band** data (except for subset of detector reset) **+ raw** data (reset pixel)

For each of the two PMD detectors, a data packet (generated every 375 ms) contains 16 readouts of 15 spectral bands (see below). The exception is the detector reset where it contains the 256 raw pixels from blocks CDE.

Transfer mode 2: **band** data (except for subset of detector reset) **+ mixed** data (reset pixel).

For each of the two PMD detectors, a data packet (generated every 375 ms) contains 16 readouts of 15 spectral bands. The exception is the detector reset where it contains 76 raw pixels (location defined in [AD9]) and 12 readouts of 15 spectral bands.

Transfer mode 3: **raw** data

For each of the two PMD detectors, a data packet (generated every 375 ms) contains the 256 raw pixels from blocks CDE. For integration times below 375 ms, only the last readout in the 375 ms period is transmitted.

A note on terminology: The name of the transfer mode is determined by the corresponding field in the Science Data Packet alone. Whether a pixel is a reset pixel or not is not relevant. Transfer mode 1 is called “band + raw”, independent of whether the ground pixel is the reset pixel or not. Do *not* consider the reset pixel in transfer mode 1 to be in “transfer mode raw”. Similarly, transfer mode 2 is always called “band + mixed“.

The 15 spectral bands are selected from blocks CDE. The pixels in each band are co-added onboard. After co-adding they are right-shifted (divided by 2), until they fit again in a 16-bit word. The co-adding factors are transmitted in status words along with the data and have to be used to reconstruct the co-added signals (module AG.5). Note that if a band is defined in block C, this band will in the nominal readout mode (1) contain meaningful data only every second readout.

For earthshine measurements, mainly band transfer (transfer mode 1 or 2) will be used, while for calibration measurements mainly raw data transfer (transfer mode 3) is foreseen.

If the calibration readout mode is selected, data have to be transmitted in the raw transfer mode. This gives the following combinations of readout and data transfer modes:

	(1) band + raw	(2) band + mixed	(3) raw
(0) nominal	yes	yes	yes
(1) solar	yes	yes	yes
(2) calibration	no	no	yes

Table 8: Possible combinations of PMD readout and data transfer modes

Every data packet reserves 304 words + 35 extra words per PMD detector. The 304 words contain:

- Band transfer: 16 readouts x (15 spectral bands + 4 status words)
- Mixed transfer: 76 raw pixels + 12 readouts x (15 spectral bands + 4 status words)
- Raw transfer: 256 raw pixels + 48 spare words

The 35 extra words will be filled with the data from block B (and 35 – Length(B) spare words *before* them).

Treatment of pixels with incomplete integration time in the GOME-2 data processor: As for the main channels, pixels with incomplete integration time shall be excluded from processing.

- In nominal and solar readout mode every second readout of block C is invalid (not completed). The PMD integration times and integration time status have no meaning in these readout modes.
- In calibration readout mode the PMD integration time status words shall be checked.

Reporting of PMD integration times in the products:

- In the products, PMD data are divided into four "bands": PMD p (blocks CDE), PMD s (blocks CDE), PMD p (block B), PMD s (block B). Integration times shall be reported for PMD p (blocks DE), PMD s (blocks DE), PMD p (block B), PMD s (block B). The integration time for block C is not reported but can easily be inferred from the PMD readout mode.

Treatment of reset pixels (nominal and solar readout mode) in the GOME-2 data processor:

- Where the processor expects band data (data co-added spectrally into 15 bands, in contrast to raw pixel data), the following data shall be discarded: in band + raw transfer mode all data from the reset pixel, in band + mixed transfer mode the raw pixel data from the reset pixel. No attempt shall be made to co-add the raw pixels from the detector reset into bands. Note that all PMD data shall be stored in the level 1a product: the above statement refers to discarding them before using them for further processing (e.g., averaging, calculation of Stokes fractions, etc.).
- It is a design feature of GOME-2 that in the reset pixel of the solar readout mode, block B signals have an additional (pixel-dependent) offset. **Data from the reset pixel of the solar readout mode shall therefore always be excluded from processing.**

Layout of 1024-element arrays for PMD data in the GOME-2 data processor and products:

- Where 1024-element arrays are used for PMD data (one 1024-element array per PMD channel), PMD raw data (and data from block B) shall be stored in the array elements corresponding to the detector pixels (see Table 6), i.e., in the last elements of the array. PMD band data shall be stored in the first 15 elements of the array.

APPENDIX C: COORDINATE SYSTEMS AND SYNCHRONISATION

This appendix outlines the conventions related to space and time coordinate systems and synchronisation issues applicable to the GOME-2 data processing. A number of applicable and reference documents ([AD7], [RD4], [RD5]) are defining conventions for coordinate systems. The subset actually used in the GOME-2 data processing is summarised here for easy reference. Furthermore, a number of GOME-2 specific issues such as scan mirror viewing angles, conventions for polarisation angles, and synchronisation aspects are discussed.

C.1 SATELLITE RELATIVE ACTUAL REFERENCE COORDINATE SYSTEM

The coordinate system used for the target directions as seen from the satellite is the *Satellite Relative Actual Reference Coordinate System*. This coordinate system is defined in the MetOp CFI Conventions document [RD5]. Its relationship to the MetOp Reference frame is explained in that document. This coordinate system is centred on the satellite in-flight centre of mass and takes into account the actual satellite orientation as described by satellite roll, pitch, and yaw angles, and any instrument specific misalignment as described by roll, pitch, and yaw mispointing angles.

Note: The term *Satellite (...)* Coordinate System is somewhat misleading: Mispointing angles are specific for each instrument. Therefore, each instrument has its own Satellite Relative Actual Reference Coordinate System.

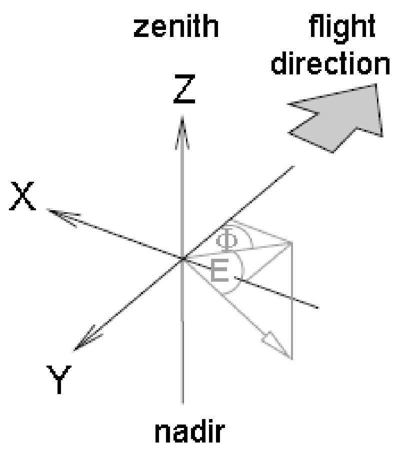

Figure 20: Satellite Relative Actual Reference Coordinate System

Specifications for this coordinate system:

- the +Z axis points vertically upwards to approximately Zenith (exactly Zenith, if all roll, pitch, and yaw angles and mispointing angles are zero),
- the +Y axis points approximately into the anti-flight direction (exactly the anti-flight direction, if all roll, pitch, and yaw angles and mispointing angles are zero), and
- the +X axis is added so that (X, Y, Z) form a right-handed coordinate system. If one sat on top of the satellite (its +Z side) and looked into flight direction (–Y), the +X direction would point to the left.

Azimuth angles ϕ are counted positive from the –Y direction via the –X direction. Elevations *E* are counted positive from the XY plane downwards (!), i.e., towards –Z.

Examples: If all roll, pitch, and yaw angles and all mispointing angles are zero, the azimuth of the –Y ("forward") direction is 0, the azimuth of the +X ("left") direction is 270°, the zenith elevation is –90°, and the nadir elevation is +90°.

Satellite zenith angles θ_s are calculated from the satellite elevation angles *E* via this formula:

$$\theta_s = E + 90°$$

Equation 403

C.2 TRUE-OF-DATE COORDINATE SYSTEM

The *true-of-date coordinate system* is used for the mean Kepler elements at ascending node crossing which are needed as input for the orbit propagation. It is defined in the EPS mission conventions document [AD7]. This system is centred on the centre of the earth and does *not* rotate with the earth. Here is a description of this system:

- the X axis points to the true vernal equinox-of-date,
- the XY plane is the true earth equatorial plane,
- the Z axis points to north.

C.3 EARTH-FIXED COORDINATE SYSTEM

The *earth-fixed coordinate system* is used for coordinates relative to the Earth's Reference Ellipsoid, in particular longitude, latitude, and altitude, but also for the orbit state vector in Cartesian coordinates. This coordinate system is defined to be the IERS Terrestrial Reference Frame in the EPS mission conventions document [AD7]. It is centred on the centre of the earth and it rotates with the earth. The following are true in this system:

- the X axis points to the Greenwich meridian (longitude zero),
- the XY plane is the true earth equatorial plane,
- the Z axis points to north.

The geodetic coordinates of a point, related to the Earth's Reference Ellipsoid WGS84, are the geocentric longitude, geodetic latitude, and geodetic altitude. The geocentric latitude is *not* used in GOME-2 processing.

Latitudes and longitudes are measured as in ISO 6709:1983. Latitude is measured negatively south of the equator and positively north, going from –90° to +90°. Longitude is measured negatively west of Greenwich and positively east, going from –180° to +180°. Should external libraries use a different convention for longitudes (measuring them from 0 to 360°), the GOME-2 processor has to convert them to the ISO 6709 representation:

$$lon_{\mathrm{ISO}} = lon_{\mathrm{external}} - 360° \quad (lon_{\mathrm{external}} \geq 180°)$$

Equation 404

C.4 TOPOCENTRIC COORDINATE SYSTEM

The *topocentric coordinate system* is used in order to specify viewing directions from a point, e.g., at the top of the atmosphere, or at scattering height, towards a target, e.g., the satellite or the sun. The viewing directions are given as azimuth and elevation angles. It is a local coordinate system centred in this point.

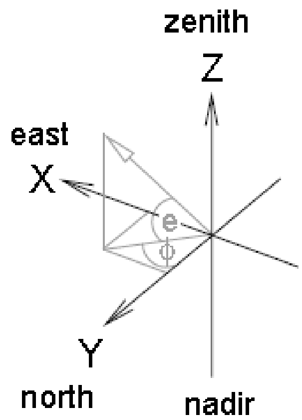

Figure 21: The topocentric coordinate system.

The topocentric coordinate system is defined in the EPS mission conventions document [AD7]. In this system:

- the X axis points to local east,
- the Y axis points to local north, and
- the Z zenith points to zenith (normal to the Earth Reference Ellipsoid).

Azimuth angles φ are counted positive from the local north direction (+Y) via the local east direction (+X). Elevations *e* are counted positive from the local horizon plane (XY) to local zenith (+Z).

Examples: The azimuth for local east is +90°, the zenith elevation is +90°, and the nadir elevation is –90°.

Topocentric zenith angles θ_t are calculated from the topocentric elevation angles *e* using the following:

$$\theta_t = 90° - e$$ *Equation 405*

C.5 SCAN MIRROR VIEWING ANGLES

The convention for GOME-2 scan mirror viewing angles corresponds to the one used in [RD1]. Referring to the Satellite Relative Actual Reference Coordinate System (see above), can mirror viewing angles ψ are measured from the –Z direction via the –X direction.

The viewing angle is zero if light from the –Z direction (approximately nadir) is entering into the optical path. The forward scan is from negative to positive viewing angles, or positive to negative X values (or from “left” to “right” using the above convention).

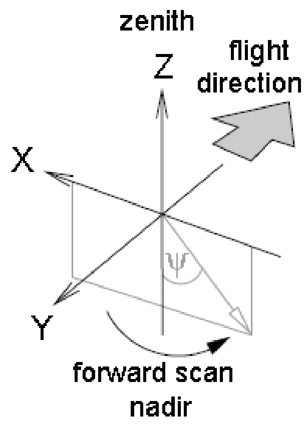

Figure 22: GOME-2 scan mirror viewing angles

Scan mirror viewing angles are derived from the scan mirror positions in the housekeeping data part of the Science Data Packet. The scan mirror position is given every 93.75 ms – 64 times per 6-second scan.

Only viewing angles (optical angles) are used in the GOME-2 processing. Rotation angles (mechanical angles) are not used at all.

C.6 POLARISATION

PMD p measures intensity polarised parallel to the spectrometer’s slit, and PMD s measures intensity polarised perpendicular to the spectrometer’s slit. The reference coordinate frame for the Stokes vectors is the local meridian plane (XZ plane in the Satellite Relative Actual Reference Coordinate System). For light fully polarised *parallel* to this reference plane (i.e., perpendicular to the instrument slit) we have a Stokes fraction $q = +1$ (maximum signal for PMD s, “no” signal for PMD p). For light fully polarised *perpendicular* to this reference plane (i.e., in Y direction, along track, parallel to instrument slit) we have $q = -1$ (maximum signal for PMD p, “no” signal for PMD s).

C.7 TIME

Unless specified otherwise, time is given as UTC, measured in fractional days since 1 January 2000, 00:00:00 hours. In order to preserve the resolution from the GOME-2 science packets (milliseconds), type double precision is required throughout for time variables. As the dating accuracy of the GOME-2 packets is not required to be better than 4 ms, the UTC word containing μ can safely be ignored. Note that in the products time will be stored as *short cds time* as specified in [AD4] and [AD5], i.e., with a resolution of 1 ms.

Note: IEEE-754 double precision uses a 52-bit mantissa which gives a precision of 2.2×10^{-16}. This is more than sufficient compared to 1 ms/25 years = 1.3×10^{-12}. On the other hand, single precision (23 bit mantissa, precision 1.2×10^{-7}) is clearly not sufficient.

C.8 SYNCHRONISATION

For a proper assignment of geolocation to the GOME-2 measurements and for a correct combination of main channel and PMD data, the synchronisation of UTC time stamps, scan mirror positions and detector readouts in the Science Data Packet has to be understood.

GOME-2 creates a Science Data Packet every 375 ms. One packet contains the following:

- one UTC time stamp t_0,
- four scanner positions (sampling 93.75 ms),
- at most two readouts of the main channels (effective integration time 187.5 ms),
- at most 16 readouts of the PMD bands (integration time 23.4375 ms).

Their relative timing is shown in Figure 23. The first scanner position is given at time $t_0 + \Delta t_{SM}$. At the same time, the first main channel readout and the first PMD readout within the packet start. The readout time is 45.78 μs per detector pixel, i.e. 46.875 ms for a complete main channel readout (1024 detector pixels), and 11.72 ms for a readout of PMD blocks BCD (256 detector pixels). Any readout operation resets a detector pixel, and therefore marks the *end* of the integration for this detector pixel. The integration starts at the *previous* readout.

The readout sequence for each detector can be programmed to be either from short to long wavelengths (“up”) or from long to short wavelengths (“down”).

How synchronisation aspects are treated in the GOME-2 data processing depends on the processing level:

- In the 0 to 1a processing, only the relative timing of UTC time stamp and scanner positions is considered (A2.3.2). Geolocation information is calculated for 187.5 ms ground pixels, independent of the actual main channel integration times and the relative timing of scanner positions and main channel readouts (A2.6).
- For the geolocation in the 0 to 1b processing (A3.2), the actual main channel integration times and the relative timing of scanner positions and main channel readouts are considered. The level 1b geolocation for a given band corresponds to the ground pixel actually covered during the integration time of this band. The finite duration of the readouts is neglected: geolocation information is given for the first detector pixel in the readout.
- For polarisation correction (A3.10) and spatial aliasing correction (A3.14) in the 0 to 1b processing, the relative timing of the main channel and PMD readouts and the finite duration of the detector readouts are accounted for.

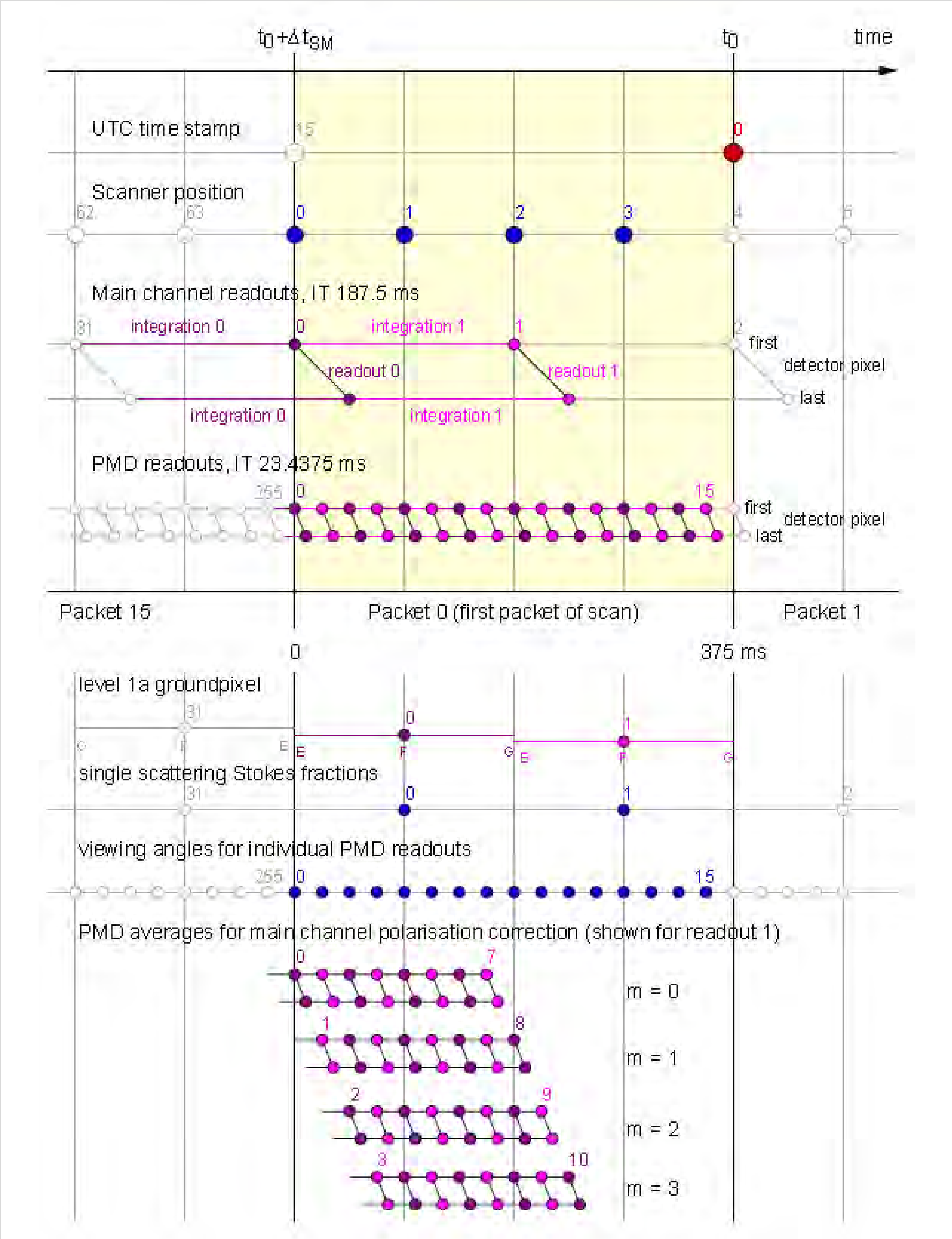

Figure 23: Synchronisation diagram. Synchronisation of time-stamp, scanner positions and detector readouts within a GOME-2 science data packet, and selected quantities of the level 0 to 1a processing. The data transmitted in packet 0 (the first of a scan) is indicated by the filled circles. Open circles belong to the previous or next data packet. For this figure, Δt_{SM} was assumed to be –375 ms. The indexing refers to a complete scan.

APPENDIX D: EXAMPLE OF A GOME-2 TIMELINE

The following preliminary table, based on photometric budget calculations, contains the different modes for the Solar calibration timeline (SOT) which is used once per day (provided by J. Callies, ESTEC):

Observation mode	***time***	***SZA***	***band 1A***	***band 1B***	***band 2A+B***	***band 3 + 4***
	(s)	degrees	(s)	(s)	(s)	(s)
	duration		240 nm - 283 nm	283 nm – 312 nm	312 nm - 400 nm	400 nm – 790 nm
dark	186		60	1.5	1.5	1.5
dark	120		1.5	0.375	0.375	0.1875
WLS	60		1.5	0.375	0.375	0.1875
dark	120		6	6	1.5	0.375
SLS	120		6	6	1.5	0.375
dark	240		1.5	0.375	0.375	0.375
sun	240		1.5	0.375	0.375	0.375
earth nadir scan	306	85	60	0.375	0.375	0.375
earth nadir scan	2223	70	12	0.1875	0.1875	0.1875
earth nadir scan	246	70	60	0.375	0.375	0.375
earth nadir scan	366	80	60	1.5	1.5	1.5
dark	306	100	60	1.5	1.5	1.5
dark	900		60	0.375	0.375	0.375
dark	651		12	0.1875	0.1875	0.1875
sum	6084					

Note: For regular nominal scanning observations, the integration times in band 1a vary between 12 and 60 seconds (i.e. comprise 2-10 scans) and that all integration times in bands 1b–4 are equal.

APPENDIX E: INSTRUMENT CALIBRATION CONSIDERATIONS

E.1. The Generic Calibration Equation

The generic expression for the signal detected by each detector pixel, as function of the incident radiation and as function of the instrument characteristics, can be written as follows:

$$S_i = I(\lambda_i) \cdot T(\lambda_i) \cdot Q_i + SS_i + DS_i$$

Equation 406

with

S_i	measured signal at detector pixel *i*
λ_i	wavelength of detector pixel *i*
$I(\lambda_i)$	incident radiation as a function of wavelength
$T(\lambda_i)$	optical transmission function of instrument as a function of wavelength
Q_i	detector efficiency (including conversion to ‘binary units’) of detector pixel *i*
SS_i	stray light at detector pixel *i* (depending on all signals in the channel)
DS_i	dark signal of detector pixel *i*

which by inversion yields this expression for the retrieved atmospheric intensity:

$$I(\lambda_i) = \frac{S_i - SS_i - DS_i}{T(\lambda_i) \cdot Q_i}$$

Equation 407

Instrument calibration comprises the determination of all quantities (except S_i) in the right-hand side of this equation.

The generic calibration equation can be rewritten as follows:

$$I(\lambda_i) = \frac{S_i - SS_i - DS_i}{c_{pol}(\lambda_i, p_t(\lambda_i)) \cdot (R_{0,i}/PPG_{0,i})(\lambda_i) \cdot PPG_{t,i} \cdot m_t(\lambda_i) \cdot E_t(\lambda_i)}$$

Equation 408

where:

subscript *0*	denotes the quantity at a reference time $t = 0$
subscript *t*	denotes the quantity at the time of measurement
$(R_{0,1}/PPG_{0,i})(\lambda_i)$	represents the smooth part of the response function as a function of wavelength, for unpolarised input
$c_{pol}(\lambda_i, p_t, (\lambda_i))$	is the polarisation correction factor as a function of wavelength and input polarisation
$PPG_{t.i}$	is the pixel-to-pixel part of the response function at detector pixel *i*
$m_t(\lambda_i)$	represents the degradation correction as a function of wavelength and
$E_t(\lambda_i)$	represents the change in Etalon as a function of wavelength

The above equation is valid for the atmospheric measurements. For the observation of the Sun there is in addition a diffuser plate (plus auxiliary optics) in the light path. The scattering properties of the diffuser plate depend both on the elevation angle of the incident beam (which is a function of time in the orbit) and on its azimuth angle (which is a function of time of the year); this two-dimensional dependency is expressed in the bi-directional scattering function (*BSDF*) of the diffuser. Noting that the sunlight is unpolarised, the generic calibration equation then takes the form:

$$I_{Sun}(\lambda_i) = \frac{S_i - SS_i - DS_i}{BSDF_0(\lambda_i) \cdot m_{BSDF,t}(\lambda_i) \cdot (R_{0,i}/PPG_{0,i})(\lambda_i) \cdot PPG_{t,i} \cdot m_t(\lambda_i) \cdot E_t(\lambda_i)}$$

Equation 409

The calibration of the instrument is performed on three different levels: on-ground calibration, performed before launch, determination of degradation M-factors, performed on approximately a monthly basis, and processing of calibration constants within the level 0 to 1a processor, performed on a timescale between one orbit and up to a few weeks (depending on the frequency of the calibration observations). The algorithms in this document are concerned with the latter item only. The other two are regarded as inputs to the processor.

E.2 INTRODUCTION TO MÜLLER MATRIX ELEMENTS

Every optical system can be described in terms of a Müller matrix which transforms an input Stokes vector (I_0, Q_0, U_0, V_0) to a Stokes vector in front of the detector (I_d, Q_d, U_d, V_d). The first element of the Stokes vector, I_0, describes the total intensity of the light. The second component, Q_0, describes the amount of linear polarisation along the X-axis of the (chosen) coordinate system. It is equivalent to the quantity $I_X - I_Y$ where I_X is the intensity of light with polarisation parallel to the X-axis and I_Y is the intensity of light with polarisation parallel to the Y-axis; note that $I = I_X + I_Y$. The third component, *U*, describes the amount of linear polarisation along the 45° direction (going from +X to +Y) of the (chosen) coordinate system. One can write $U = I_{45°} - I_{135°}$.

Note: *I* can also be written as follows: $I = I_{45°} + I_{135°}$.

Although not further needed in this section, it is mentioned that the total amount of linearly-polarised light, P, and the polarisation angle, χ, are given by the following:

$$P = \sqrt{(Q_0/I)^2 + (U_0/I)^2} \text{ and } \chi = \text{atan}(U_0/Q_0)$$

See Section 5.2.23for a detailed explanation.

Unlike Q_0 and U_0 , the quantity P is independent of the choice of coordinate frame.

The last component of the Stokes vector, V_0, describes the amount of circularly polarised light. For the radiation from the Earth's atmosphere, Stokes element V_0 is expected to be very small, and the Müller matrix elements of the GOME-2 instrument which could mix V_0 into I_d are small enough that we can neglect V_0 altogether.

The radiation transfer through the instrument can then be written in the form:

$$\begin{pmatrix} I_d \\ Q_d \\ U_d \end{pmatrix} = \begin{pmatrix} M^1 & M^2 & M^3 \\ \dots & \dots & \dots \\ \dots & \dots & \dots \end{pmatrix} \cdot \begin{pmatrix} I_0 \\ q_0 \\ u_0 \end{pmatrix}$$

Equation 410

where $q = Q/I$ and $u = U/I$. Since the detector only measures intensity (its quantum efficiency is independent of polarisation) the first row of the Müller matrix is the only significant one. Therefore, the signal S of any detector in GOME-2 (channel array or PMD) can be expressed as follows:

$$S = M^1 \cdot I_0 + M^2 \cdot Q_0 + M^3 \cdot U_0 = M^1 \cdot I_0 \cdot \left\{ 1 + \frac{M^2}{M^1} \cdot q + \frac{M^3}{M^1} \cdot u \right\}$$

Equation 411

where the matrix elements now implicitly include the detector efficiency and electronics amplification. The task of level 1 processing is to invert this equation and derive the intensity I_0 from the signal. This needs the on-ground calibration of the matrix elements, and the determination of the Stokes fractions q, u.

E.3 COMPARISON OF EXPRESSIONS FOR INSTRUMENT CALIBRATION

In this subsection we compare the calibration equations from the GOME-2 calibration plan [RD 2] with the equations in terms of MMEs. The various calibration equations may be compared to the generic calibration equation introduced in equation (409). The GOME-2 calibration plan [RD 2] describes the calibration of the instrument directly in terms of the calibration Key Data. Polarisation is described using the fraction of light polarised parallel to the spectrometer's slit. This polarisation parameter is denoted p and is, depending on the chosen coordinate frame, a simple transformation of the Stokes fraction q:

$$p = 0.5 \cdot (1 - q)$$

Equation 412

The PMD-p measures the polarisation in a direction parallel to the instrument slit; light fully polarised in this direction is referred to as 'p-polarised' light and has $p = 1$. The PMD-s measures the polarisation in a perpendicular direction; light fully polarised in this direction is referred to as 's-polarised' light and has $p = 0$. The atmospheric radiance *I0* is calculated from the signal *S* (corrected for dark signal and stray light) by the following expressions.

According to [RD 2] we can write in simplified form (ignoring wavelength- and scan angle dependencies):

$$I_0 = \frac{S}{R_u \cdot c_{pol}} \quad \text{with} \quad c_{pol} = \left[0.5 \cdot \frac{1+\eta}{(1-\eta)\cdot p + \eta}\right]^{-1}$$

Equation 413

where η is the ratio of (response to s-polarised light)/(response to p-polarised light) and R_u is the response to unpolarised light.

The polarisation fraction *p* is calculated from the PMDs via this equation:

$$p = \frac{1}{1 + \frac{Z}{A}} \quad \text{with} \quad Z = \frac{S(\text{s-pmd})}{S(\text{p-pmd})}$$

Equation 414

and α is the value of *Z* for the on-ground calibration using unpolarised light.

The calibration Key Data are the variables [R_u η α]. According to the Müller matrix formalism the calibration expression is as follows:

$$I_0 = \frac{S}{M^1 \cdot c_{pol}} \quad \text{with} \quad c_{pol} = 1 + \mu 2 \cdot q$$

Equation 415

The Stokes fraction *q* is calculated from the PMDs via this formula:

$$q = \frac{\alpha - Z}{\alpha + Z} \quad \text{with} \quad Z = \frac{S(\text{s-pmd})}{S(\text{p-pmd})}$$

Equation 416

The Müller matrix elements are the variables [M^1 $\mu 2$ α] which can be easily derived from the Calibration Keydata of [RD 2] using this formula:

$$M^1 = R_u \text{ and } \mu 2 = \frac{1-\eta}{1+\eta}$$

Equation 417

Note: This transformation needs to be made only once as a preprocessing step.

E.4 POLARISATION PHASE SHIFT

The formulations for the calculation of polarisation as presented in Section 5.2.3 hold for an ideal instrument with all optics perfectly aligned and without any polarisation shift problem (i.e. a mixing of p-polarised light into s-polarised light and vice versa within the instrument). In the case of a polarisation phase shift, the Müller matrix formalism can be easily expanded. In this case we get the following:

$$I_0 = \frac{S}{M^1 \cdot c_{pol}} \quad \text{with} \quad c_{pol} = 1 + \mu 2 \cdot q + \mu 3 \cdot u$$

Equation 418

In this case a new calibration parameter $\mu 3 = \frac{1-\zeta}{1+\zeta}$ is needed. The parameter ζ will be measured during calibration. It can be shown that the solution in the Müller matrix formalism can be written as follows:

$$q = \frac{\alpha - Z}{\rho \cdot Z - \sigma \cdot \alpha}$$

Equation 419

where, without phase shift, we have ρ = +1, and σ = -1 with phase shift; the variables ρ and σ contain the polarisation ratio *u/q* which can for each ground pixel be estimated from theoretical calculations of atmospheric Rayleigh scattering as described in Section 5.2.23.

APPENDIX F: PRELIMINARY HOUSEKEEPING DATA CONVERSION COEFFICIENTS

In the absence of [AD6], preliminary coefficients HK^m for conversion of instrument housekeeping data to physical units for use in module AG.4 are given below. They are suitable for use in prelaunch processor testing. However, for operational processing of post-launch data they *must* be replaced by values valid for the respective GOME-2 flight model as specified in [AD6]. ***Note***: The conversion is linear, i.e., $HK^m = 0$ for $m = 2, 3, 4$.

Parameter	*SDP word*	HK^0	HK^0	*Units*	*Remarks*
WLS voltage	50	–0.1159684	7.62939×10^{-4}	V	
WLS current	51	-1.426716×10^{-3}	7.62939×10^{-6}	A	
SLS voltage	52	–1.464864	7.62939×10^{-3}	V	
SLS current	53	0	7.62939×10^{-7}	A	
FPA array temperatures	54-85	0.16	$7.62939 \cdot 10^{-3}$	K	
Peltier output	86-101	0	0.025	V	
Scan mirror position	106-109	–98.5694	$360 / 2^{15}$	degree	$\psi_{SM,m}$, used in module A2.3
Scan mirror torque	110-113	–1000	0.48828	Nm	
Radiator temperature	343	0.16	7.62939×10^{-3}	K	
WLS DC/DC temperature	347	100.2618	5.249×10^{-3}	K	valid only if WLS is ON
SLS DC/DC temperature	349	52.5253	6.382×10^{-3}	K	valid only if SLS is ON
Centre of OB temperature	353	0.16	7.62939×10^{-3}	K	
Predisperser temperature	357	0.16	7.62939×10^{-3}	K	
PMD array temperature	368 – 369	0.16	7.62939×10^{-3}	K	
other temperatures	various	0.16	7.62939×10^{-3}	K	

Table 9: Housekeeping data conversion coefficients for use in processor testing as extracted from the GOME-2 FM3 database in September 2003.

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