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Algorithm theoretical basis document for the TROPOMI L01b data processor



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Authors

Ljubiša Babić	Remco Braak	Werner Dierssen
Jonathan Kissi-Ameyaw	Quintus Kleipool	Jonatan Leloux
Erwin Loots	Antje Ludewig	Nico Rozemeijer
Joost Smeets	Giuseppe Vacanti	

with contributions from:

Airbus Defense and Space The Netherlands¹
Netherlands Organisation for Applied Scientific Research TNO
SRON Netherlands Institute for Space Research

¹ formerly know as Dutch Space B.V. The Netherlands

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1 Introduction

1.1 Identification

This document, identified as CI-6480-ATBD, contains the theoretical algorithmic basis of the Level-0 to Level-1b data processing for the TROPOMI mission. This ATBD gives the highest level description of the algorithms used in the Level-0 to 1b data processing and as such, provides criteria that are used to validate and accept the software.

The TROPOMI Level-0 to Level-1b data processor (L01b) is developed by the Royal Dutch Meteorological Institute (KNMI) under contract of the National Space Organization (NSO). The extent and scope of this work is described in the Software Development Plan for TROPOMI L01b data processor (SDP) [AD1]. This document is a constituent of the KNMI TROPOMI Technical Baseline File, as defined in Software Product Assurance Plan (SPAP) [AD2].

1.2 Purpose and objective

This document contains a detailed description of the TROPOMI instrument and the algorithms incorporated into the L01b Processor. The purpose of this document is to give the theoretical basis for the algorithms needed to convert Level 0 data to Level 1b data. Note that the derivation of the calibration key data delivered by the calibration program will not be described here: these key data are considered given entities here. In addition, this document aims at providing users of L1b and L2 with a concise description of the instrument, the processor data products, as well as the assumptions under which they were generated, and any limitations associated with them.

The SDP and SPAP are applicable to this ATBD but since these do not contain any requirements, they are not parent documents and there is no tracing to these documents. The S5P Systems Requirements Document (SRD) [RD4] only contains a few requirements that are applicable to the L01b Processor. However, this SRD does not cover the required functionality of the L01b Processor in full and therefore, cannot act as a “full parent”. In order to solve this problem, the functional requirements of the SRD are covered in the System Software Specification (SSS) [RD5], whereas the requirements related to quality are covered in the Scientific Quality Requirements Document (ScQRD) [AD3]. Both documents contain many new requirements that cannot be traced to higher-level documents. The ScQRD demonstrates that the SRD requirements can be met from an error budget point of view. The algorithms in the ATBD have been developed with this error partitioning in mind. As such, the ATBD is considered to be a child of the ScQRD. Together the SSS, ScQRD and ATBD documents serve as the top level requirements specification for the L01b Processor.

Examining the previous point in more detail, there are several rationales for the specification sharing between these documents: first, the quality and accuracy requirements will be verified and validated using an independent method to that of the verification and validation program for the SSS specific requirements (see SDP and SPAP); second, it will make both the ATBD and SSS easier to manage; and third, it is expected that the algorithms be subject to change until late in the development of the L01b Processor, whereas the SSS requirements are likely to be far more stable. Further, separating the SSS and ATBD will allow the SSS requirements to be frozen early on in the program, whilst keeping the required flexibility for algorithm changes in the ATBD.

1.3 Document overview

The ECSS standards do not provide a Document Requirements Definition (DRD) for the ATBD. This document therefore follows the KNMI documentation model as defined in [RD6]. The first three sections provide the standard information necessary for document context: Section 1 - Introduction; Section 2 - Applicable standard and reference documents; Section 3 - Terms, definitions and acronyms used in the document.

The remainder of the document is split into seven parts: Part I gives the top level overview of the mission and how the L01b Processor relates to the overall program, calibration, and the ground segment (Section 4). It also provides some important notes on error propagation and (Section 5) as well as some specific conventions used throughout this document (Section 6).

Part II contains the instrument description with the optics in Section 7, the detectors in Section 9, the instrument control unit in Section 8 and some details on assumed straylight performance in Section 10.

Part III contains the operational aspects relevant to TROPOMI L01b processing, with the orbit definition in Section 11, some notes on instrument operations in Section 12, the instrument modes in Section 13, instrument calibration in Section 14, and data processing in Section 15.

Part IV contains the forward model. This mathematically describes how the signal is transformed as it enters the telescope, interacts with the optics and detectors, before being passed to the spacecraft systems for transmission to the ground segment. The optics are detailed in Section 16, the detectors in Section 17, and the electronics in Section 18.

Part V contains the instrument reverse model. This describes the computational model responsible for correcting and calibrating satellite telemetry in order to give an estimate of the input signal and its variance. After a discussion of the processing flow (Section 19) and some general remarks on data propagation (Section 20), there are two sections on generic corrections (Section 21 and 24) that are valid for both the UVN and the SWIR modules. In addition, the module specific corrections are given in Section 22 and 23 for the UVN and SWIR module, respectively.

Part VI gives information on all measurement annotation foreseen for L01b processing. This includes time bases in Section 25, geometrical definitions in Section 26, geometrical algorithms in Section 27, wavelength characterization in Section 28, and quality assessment in Section 29.

Mathematical reasoning and calculations with respect to the use of Chebychev polynomials, the use of small-pixel data, and the convolution of the slit function with the solar irradiance spectrum are contained in the appendices in Part VII at the end of the document.

2 Applicable and reference documents

2.1 Applicable documents

- [AD1] Software development plan for TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0002-PL; **issue:** 2.0.0; **date:** 2012-11-14.
- [AD2] Software product assurance plan for TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0003-PL; **issue:** 2.0.0; **date:** 2012-11-14.
- [AD3] Scientific quality requirements document for TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0008-RS; **issue:** 3.0.0; **date:** 2013-06-26.

2.2 Reference documents

- [RD4] GMES Sentinel-5 Precursor system requirement document.
source: ESA; **ref:** S5p-RS-ESA-SY-0002; **issue:** 4 rev. 1 – Redlined Version - RLa; **date:** 2011-04-29
–Redlined version: 2012-07-04.
- [RD5] Software system specification for TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0005-RS; **issue:** 3.0.0; **date:** 2012-11-21.
- [RD6] KNMI standards and procedures for the TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0001-PL; **issue:** 2.0.0; **date:** 2012-05-10.
- [RD7] Terms, definitions and abbreviations for TROPOMI L01b data processor.
source: KNMI; **ref:** S5P-KNMI-L01B-0004-LI; **issue:** 3.0.0; **date:** 2013-11-08.
- [RD8] J. P. Veefkind, I. Aben, K. McMullan *et al.*; TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. *Remote Sensing of Environment*; **120** (2012), 70; 10.1016/j.rse.2011.09.027.
- [RD9] S5P TROPOMI nominal operations baseline.
source: KNMI; **ref:** S5P-KNMI-OPS-0056-TN; **issue:** 5.0.0; **date:** 2016-01-22.
- [RD10] Calibration requirements specifications for the TROPOMI in-flight calibration.
source: KNMI; **ref:** S5P-KNMI-ICAL-0006-RS; **issue:** 1.0.0; **date:** 2014-10-28.
- [RD11] Algorithm theoretical basis document for TROPOMI UVN on-ground calibration key data calculation.
source: KNMI; **ref:** S5P-KNMI-OCAL-0005-SD; **issue:** 3.0.0; **date:** 2016-04-01.
- [RD12] Algorithm theoretical basis document for TROPOMI SWIR on-ground calibration key data calculation.
source: SRON; **ref:** SRON-S5P-OCAL-SP-002-ATBD; **issue:** 2.0.0; **date:** 2016-04-01.
- [RD13] Department of Defense World Geodetic System 1984.
source: NIMA; **ref:** NIMA TR8350.2; **issue:** Third Ed.; **date:** 2000-01-03.
- [RD14] IERS Technical Note No. 36 - IERS Conventions (2010).
source: IERS; **ref:** IERS Technical Note No. 36.
- [RD15] Supplement to Department of Defense World Geodetic System 1984 Technical Report: Part I - Methods, Techniques, and Data Used in WGS84 Development.
source: DMA; **ref:** DMA TR 8350.2-A; **issue:** Second Printing; **date:** 1987-12-01.
- [RD16] Toshio Fukushima; Transformation from Cartesian to geodetic coordinates accelerated by Halley's method. *Journal of Geodesy*; **79** (2006), 689; 10.1007/s00190-006-0023-2.
- [RD17] Sean E. Urban and P. Kenneth Seidelmann (editors) *Explanatory Supplement to the Astronomical Almanac* (University Science Books, 2013); 3rd edition.
- [RD18] T. C. van Flandern and K. F. Pulkkinen; Low-precision Formulae for Planetary Positions. *Astrophysical Journal Supplement Series*; **41** (1979), 391.
- [RD19] J. Meeus; *Astronomical Algorithms* (Willman-Bell, Inc., 1998); 2nd edition; ISBN 0-943396-61-1.

- [RD20] Sentinel-5 UVNS Instrument Phase A/B1 Reference Spectra.
source: ESA; **ref:** IPD-RS-ESA-18; **issue:** 1 rev. 2; **date:** 2011-02-10.
- [RD21] C. Caspar and K. Chance; GOME wavelength calibration using solar and atmospheric spectra. *In Proceedings of the third European Remote-Sensing Satellite Scientific Symposium: Space at the service of our environment* (edited by T.-D. Guyenne and D. Danesy); volume SP-414; (pp. 609–614) (European Space Agency, Noordwijk, The Netherlands, 1997).
- [RD22] J. H. G. M. Van Geffen and R. F. van Oss; Wavelength calibration of spectra Measured by the Global Ozone Monitoring Experiment by use of a high-resolution reference spectrum. *Applied Optics*; **42** (2003) (15), 2793; 10.1364/AO.42.002739.

2.3 Electronic references

- [ER23] <http://eclipse.gsfc.nasa.gov/SEcat5/SE2001-2100.html>.

3 Terms, definitions and abbreviated terms

Terms, definitions and abbreviated terms that are used in development program for the TROPOMI L01b data processor are described in [RD7]. Terms, definitions and abbreviated terms that are specific for this document can be found below.

3.1 Terms and definitions

There are no document specific terms and definitions.

3.2 Acronyms and abbreviations

BOL	Beginning-Of-Life
CIO	conventional international origin
CIP	celestial intermediate pole
EFRF	Earth-fixed reference frame
EOL	End-Of-Life
FK5	Fifth Fundamental (star) Catalogue
GCRS	IERS geocentric celestial reference system
GMT	Greenwich mean time
GST	Greenwich sidereal time
IAU	International Astronomical Union
ICU	instrument control unit
IERS	International Earth Rotation and Reference Systems Service
IRF	inertial reference frame
IRM	IERS reference meridian
IRP	IERS reference pole
ITRF	IERS terrestrial reference frame
ITRS	IERS international terrestrial reference system
J2000.0	12:00 (noon), 1st of January 2000 UT1
LNP	local normal pointing
LORF	local orbital reference frame
LRORF	local relative orbital reference frame
OAC	optical alignment cube
OARF	optical alignment reference frame
ORF	optical reference frame
PRF	payload reference frame
ROIC	read-out integrated circuit
SRF	spacecraft/satellite reference frame
TIRS	terrestrial intermediate reference system
TRF	topocentric reference frame
TT	terrestrial time

Part I

Top level overview

In this part, we give a top level overview of the TROPOMI instrument and its L01b Processor, including the objective of the mission, the philosophy on noise and errors, and some conventions used in the document. [RD8] served as a source for the mission objective section.

4 Mission objective

4.1 Copernicus and GMES

Copernicus – previously known as GMES² – is the European programme for the establishment of a European capacity for Earth Observation and is a joint initiative of the European Community and the European Space Agency ESA. The overall objective of the initiative is to support Europe's goals regarding sustainable development and global governance of the environment by providing timely and high quality data, information, services and knowledge. The Declaration on the GMES Space Component Programme states that the Sentinel-5 Precursor (S5p) mission will be implemented as part of the initiative.

The S5p mission is a single-payload satellite in a low Earth orbit that provides daily global information on concentrations of trace gases and aerosols important for air quality, climate forcing, and the ozone layer. The payload of the mission is the TROPOspheric Monitoring Instrument (TROPOMI), which is jointly developed by The Netherlands and ESA. The instrument consists of a spectrometer with spectral bands in the ultraviolet, the visible, the near-infrared and the shortwave infrared. The selected wavelength range for TROPOMI allows observation of key atmospheric constituents, including ozone (O₃), nitrogen dioxide (NO₂), carbon monoxide (CO), sulfur dioxide (SO₂), methane (CH₄), formaldehyde (CH₂O), aerosols and clouds.

4.2 Mission planning

With a planned launch date of April 2016 and a lifetime of seven years, S5p provides high spatially resolved observations of trace gases in the period between the current Ozone Monitoring Instrument OMI and SCIAMACHY³ observations, and the upcoming operational Sentinel-5 observations starting around 2020. In addition, the early afternoon observations of TROPOMI have strong synergy with the morning observations of GOME-2 (Global Ozone Monitoring Experiment 2). Although GOME-2 has a lower spatial resolution and does not include the SWIR spectral range, the combination of TROPOMI and GOME-2 allows observing diurnal variations, as successfully shown with the OMI-SCIAMACHY combination. The combination of TROPOMI and GOME-2 is a first step toward higher temporally resolved observations over Europe starting in 2019 with the Sentinel-4 mission on the geostationary MTG (Meteosat Third Generation) sounder platform.

In addition to the GOME-2 synergy, there is also a synergy between TROPOMI and the U.S. NPP (Suomi National Polar-orbiting Partnership) satellite. Identified synergies include the use of the VIIRS (Visible/Infrared Imager Radiometer Suite) for high spatially resolved cloud information and OMPS (Ozone Monitoring and Profiling Suite) for high vertically resolved stratospheric ozone profiles. It is planned to fly the S5p mission within approximately 5 minutes of NPP, thus building upon the successes of the "A-Train" constellation of Earth observation satellites.

S5p/TROPOMI will not only continue the GOME (since 1995), OMI and SCIAMACHY data records, but also make an important step toward the challenging Sentinel-5 requirements. The high spatial resolution of TROPOMI of $7 \times 7 \text{ km}^2$ at nadir is a major step forward and allows for the detection of small-scale sources and will increase the fraction of cloud-free observations by an estimated 70 % as compared to OMI. The high spatial resolution requirements for the Sentinels-4 and 5 cannot be fulfilled with GOME-2, which nominally has a spatial resolution of $80 \times 40 \text{ km}^2$. Furthermore the CO and CH₄ observations from thermal infrared sounders like IASI (Infrared Atmospheric Sounding Interferometer) provide little information in the boundary layer.

4.3 Orbit rationale

The early afternoon orbit has been recommended for the S5p mission for the following reasons:

² Global Monitoring for Environment and Security ³ Scanning Imaging Absorption spectroMeter for Atmospheric CartographY

- In the afternoon the boundary layer is well developed and is representative for the build up of pollution emitted during daytime, when most anthropogenic activity takes place.
- From a timeliness perspective, the data of the early afternoon are the last that can be used for air quality forecast and warnings for the next day.
- In the timeframe 2016 – 2020, the S5P TROPOMI afternoon observations will be complementary to the MetOp GOME-2 and IASI morning observations, thus providing two observations (more at higher latitudes) during the day. Having more than one observation per day will aid the development of tools required for the Sentinel-4 mission, that will provide hourly observations over Europe during daytime.
- The early afternoon orbit provides the opportunity to use the synergy with the U.S. NPP satellite, which can provide high spatial resolution information on clouds and aerosols, as well as ozone profile information with high vertical resolution in the stratosphere.
- The selected orbit has about the same local overpass time as OMI on EOS Aura, which is beneficial for detecting trends in the combined OMI/TROPOMI data record.

4.4 Payload

S5P is a single satellite, single payload intermediate-stage mission, acting as a preparatory program for Sentinel-5 on the EUMETSAT Polar System (EPS) Second Generation. The S5P mission will fill the gap between the end of the OMI and SCIAMACHY exploitation and the start of the Sentinel-5 mission. In view of the transitional nature of the Sentinel-5 Precursor Mission, key programmatic constraints are a short development time and limited budget, therefore demanding a heavy reliance on national developments and experience.

The S5P technical definition is based on national studies in The Netherlands, Sentinel-4/5 studies and complementary activities addressing topics such as suitable (small) platforms. It takes national developments into account, particularly those under the TROPOMI program, and iterates between design activities and requirement analysis, supported by expert groups. The starting point is represented by the observation requirements defined in the GMES Sentinel-4/5 Mission Requirements Document (MRD) (ESA, in preparation). In line with the relevant provisions of the Declaration on the GMES Space Component Program, ESA's undertaking foresees the development of a satellite system encompassing the spacecraft, accommodation of the TROPOMI payload (jointly developed by The Netherlands and ESA), a basic ground segment and the launch and in-orbit commissioning.

4.5 Launcher

A dedicated launcher of the ROCKOT class will be used to inject the S5P spacecraft directly into its final orbit in April 2016 and the in-orbit lifetime of the spacecraft is seven years. The S5P reference orbit is a near-polar frozen sun-synchronous orbit, adopted for mission optimization with a mean local solar time at ascending node (LTAN) of 13:30 h and a repeat cycle of 17 days. The orbital height is nominally 824 km, and has been selected so as to fly in formation with the U.S. NPP mission.

4.6 Ground segment

The ground segment for S5P will consist of a Flight Operations Segment (FOS), Payload Data-processing Ground Segment (PDGS) and Mission Planning Facility (MPF). The TROPOMI Level 0-1b software will be provided by The Netherlands and installed in the PDGS. The Level 1 - 2 software is expected to have both national and Copernicus programme contributions. The FOS consists of hardware and software necessary to uplink commands and process down-linked housekeeping telemetry from the satellite. It will also house the Operational Command and Telemetry Databases, derived from the Spacecraft Reference Database. The PDGS will execute systematic nominal processing of all down-linked payload data, either locally or remotely. During the launch and early orbit phase (LEOP), the network of ground stations will be enhanced and stations added for extra control of the spacecraft. These elements of the ground segment should ensure that near real-time availability of many of the TROPOMI products, within three hours of on-board capture.

4.7 Relation to calibration

For the retrieval of absolute densities of atmospheric constituents, the TROPOMI instrument needs to be calibrated with respect to known radiometric sources prior to launch. During the operational phase relative calibrations using the Sun as a source are performed.

Calibration measurements are used to derive calibration key data parameters that are required for the L01b processor to compute absolute radiance values from the raw instrument data. During the on-ground calibration of the TROPOMI instrument, the L01b processor is also employed to determine calibration key data parameters (CKDs) from the calibration measurement data. This ensures that a consistent set of CKDs are derived. Furthermore the processor is used to verify and validate the CKDs. This is achieved by reprocessing the measurement data, analyzing the remaining uncorrected effects and determining the calibration key data parameters independently from different data sets. The use of the L01b processor ensures that the same algorithms are used for all data and no additional sources for errors and inconsistencies are introduced. The L01b Processor also computes the error and the noise associated with the processed signal (see Section 5). This has the advantage that an error margin is attached to all calibration key data parameters. The compliance with requirements on accuracy can thus be validated almost immediately.

5 Philosophy on noise and errors

The leitmotiv of this document is the tension between what we know about the instrument and the physics, and our understanding and apprehension of the observations that the instrument generates. The three large parts in this document, the instrument description, the forward model and the reverse model, reflect this tension. The instrument transforms the signals we want to know, i.e. irradiance and radiance, into mere digital numbers. This process is described in the forward model, which in turn makes use of the combined understanding of the instrument (described in the instrument model) on the one hand and physics on the other hand. The reverse model describes our attempt to invert, as completely as possible, the forward path of the signals. The resulting *reconstructed* radiance and irradiance signals should be viewed with this thought in mind. In order to obtain a better grasp of the caveats involved, we formally divide the level 1b product into three parts. This will be explained below.

5.1 Signal, noise and error

It is important to make a strict distinction between noise and error.

5.1.1 Error

The reverse model is implemented in the L01b Processor: a set of consecutive algorithms that transforms a specific measured signal leaving the instrument back towards (ir)radiance entering the instrument.

During this process, *errors* can be introduced at every step. A specific pixel on the ground is observed only once, under specific illumination conditions. The radiance at the entrance of the instrument is transformed in one digital number, that has no associated error. The processor will apply the required corrections to that digital number to arrive at the best estimate of the photon count at the entrance of the instrument. In this process, two kinds of errors are made.

Algorithm errors Each algorithm in the processor is associated with some step in the forward model. In an ideal situation, the algorithm applies exactly the inverse operation as the associated forward step. For example, an offset that is added to the signal in the forward model is corrected in the reverse model by subtracting the same offset. In this example, the inverse operation can be described exactly and no information is lost. However, some steps in the forward model involve information loss by reducing data (binning, co-addition). Other steps are in theory deterministic and therefore invertible while in practice some approximations and discretizations have to be made (e.g., in the case of straylight). Further, numerical errors can occur. Examples are long computations that cause loss of significance (like algorithms for computing standard deviations) and matrix inversion by iterative methods.

Calibration errors Most (but not all) correction steps consist of applying additive or multiplicative operations to the signal. The terms and factors have been acquired from on-ground and in-flight calibration. These

so-called calibration key data parameters (CKDs) contain errors. These errors can originate from measurement noise (more on this below) or from the calibration algorithms that extract the CKD from raw measurement data. Calibration errors can operate on different scopes. The error on gain ratio affects the entire measurement while an error in pixel-response non-uniformity (PRNU) is pixel-dependent.

Whatever their origin, the calibration and algorithm errors are systematic in the sense that they operate on each input signal and they will change a signal. If a particular signal is fed twice to the processor, the calibration errors will change the signal in exactly the same way. In the reverse model, we can calculate the associated variance due to the various calibration and algorithm errors in each step. These systematic errors are propagated together with the signal. Note that at the start, before any algorithm has been applied, the signal has no variance.

5.1.2 Noise

Now consider the situation that a ground pixel has been measured several times. Each of the digital numbers is propagated through the reverse model, acquiring propagated variances stemming from the same systematic algorithm and calibration errors. However, these digital numbers at the start are not the same. This is due to *measurement noise*, or noise in shorthand. The idea is that an estimate of the noise is provided together with a single signal measurement. This is not quite a contradiction: we repeat that an individual measurement contains no noise. However, theory and/or associated measurements give information of the noisiness of the signal. Measurement noise is, stemming from two physical sources, split into two terms: read-out noise and shot noise.

Read-out noise Read-out noise is a consequence of the imperfect operation of the physical electronic detector chain. This involves the whole process from the incidence of photons on the detector pixel, the amplifiers, the conversion from electrons to volts to digital numbers. The read-out noise does not depend on the magnitude of the signal. Read-out noise can be injected in the reverse model in two ways:

- It is actually a CKD in itself; it is a by-product of the offset determination calibration algorithm. The variations of the offset in the same picture during several measurements provide the estimate of the read-out noise.
- The current measurement, containing thousands of pixels, can provide information about the read-out noise from a subset of these pixels with known behavior.

Once the estimate has been made, somewhere in the processing chain, it has to be transferred through the conversion steps in order to compare it with the resulting (ir)radiance signal.

Shot noise Shot noise exists because light and electric current consist of the movement of discrete 'packets'. These packets are photons in the case of light and electrons in the case of electric current. Light coming from the Sun hits a detector pixel, which creates an electric charge. The fundamental physical processes that govern light emission are such that these photons are emitted from the Sun at random times; but the many billions of photons are so many that the brightness of the Sun, expressed as the number of photons per unit time, varies only infinitesimally with time.

However, if the amount of light and the size of the receiving pixel is small, only a moderate amount of photons hit the specific pixel every second. Thus the relative fluctuations in number of photons, i.e. the signal received by the detector pixel will be significant, just as when tossing a coin a few times. These fluctuations are shot noise. The process is adequately described by a Poisson distribution. The standard deviation of the shot noise is equal to the square root of the number of electrons generated. This shot noise transfers through the correction steps in the reverse model. Details follow in Section 20.2.

5.1.3 Summary

To summarize, the processor provides for each measurement the following three quantities:

- The signal, as reconstructed by the algorithm chain, in radiance/irradiance units.
- The error, stemming from calibration and algorithm errors, propagated through the same chain using formal error propagation rules and expressed in the associated radiance/irradiance units

- The noise, consisting of shot noise and read-out noise, converted to the radiance/irradiance units. In Section 20.2, the propagation of the two measurement noise terms is further explained.

6 Conventions

6.1 Units

This document generally employs the international system of units (SI). Notably, numbers of photons are expressed in mol, which complies with the NetCDF climate and forecast (CF) metadata convention. On the other hand, numbers of electrons are expressed in electrons (symbol e^-), which is not an SI unit and therefore does not comply with CF. This is however no problem as this unit is only used internal to the L01b Processor. Dimensionless parameters are listed as having unit 1. This is to distinguish from enumerating parameters (such as spectral band), which are listed as having no applicable unit.

6.2 Mathematical conventions

Enumerators TROPOMI has four detectors, which are numbered $d = 1, 2, 3, 4$. Since d is one of the enumerating parameters referred to in Section 6.1, arithmetic operations on d are meaningless. Therefore, it is also acceptable to ‘number’ $d = \text{UV, UVIS, NIR, SWIR}$, respectively. Each of the detectors is divided in two, giving a total of eight spectral bands, numbered $b = 1, \dots, 8$. b is another enumerating parameter.

Iterators Since the TROPOMI detectors are two-dimensional, consisting of pixels on a rectangular grid, many concepts in the L01b Processor (including the measured signal) are presented as matrices. Rows and columns of such a matrix are numbered using the iterating parameters r and c , respectively. Further, we often use the symbol \mathbf{x} as a shorthand for r, c . Such matrices may be binned (where groups of pixels are aggregated, leading to a smaller-sized matrix) or unbinned (where such adding has not occurred and the matrix has the maximum size). In the former case, we speak of ‘image pixels’, \mathbf{x}_{img} , r_{img} , and c_{img} . In the latter, we speak of ‘detector pixels’, \mathbf{x}_{det} , r_{det} , and c_{det} .

Matrix indexation To reduce the amount of subscripts in mathematical equations and thus improve their readability, we sometimes use square brackets to denote elements of vectors or matrices, i.e., $M[i, j]$ for M_{ij} , especially if the indexes themselves have subscripts. Therefore, the signal S of a particular detector pixel is denoted as $S[r_{\text{det}}, c_{\text{det}}]$. Using the shorthand \mathbf{x} , a summation over an area A on the detector is now easily expressed as a single summation,

$$\sum_{\mathbf{x}_{\text{det}} \in A} S[\mathbf{x}_{\text{det}}] .$$

A specific application of this notation is in binning an unbinned parameter. For instance, the value of a parameter c for an image pixel \mathbf{x}_{img} is expressed in the corresponding values for the detector pixel \mathbf{x}_{det} as

$$c[\mathbf{x}_{\text{img}}] = \frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} c[r_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} ,$$

where $\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}$ denotes the set of detector pixels that corresponds with one image pixel.

Alternative arctangent function Some of the geometrical algorithms need a mathematical function that returns the angle between a vector (x, y) and the X -axis in 2-dimensional space. Since this is similar to the arctangent function, we denote this function arctan2 analogous to the corresponding function that is found in some computer languages. The relation between the two functions is given by:

$$\text{arctan2}(x, y) = 2 \arctan \frac{y}{\sqrt{x^2 + y^2} + x} .$$

Note that the arctan2 function gives values between $-\pi$ and $+\pi$ while the arctan function gives values between $-\pi/2$ and $+\pi/2$. However, the function is not defined for $y = 0, x < 0$ and may overflow around these regions, and gives an error for $\text{arctan2}(0, 0)$. This has to be taken into account when implementing this equation.

6.3 Correction algorithms

The correction algorithms described in Part V usually consist of the four simple arithmetic operations of addition, subtraction, multiplication, and division. Of these, addition and subtraction are equally efficient for a computer

program. However, division is computationally less efficient than multiplication. Therefore, the division of a matrix by a constant value is written as a multiplication of the matrix by the reciprocal of that constant value. That way, the division has to be carried out only once.

Part II

Instrument description

The TROPOMI instrument (TROPOMI) is a space-borne nadir-viewing hyperspectral imager with four separate spectrometers covering non-overlapping and non-contiguous wavelength bands between the ultraviolet and the shortwave infrared. The purpose of TROPOMI is the measurement of atmospheric properties and constituents. The instrument uses passive remote sensing techniques to attain its objective by measuring at the top of the atmosphere the solar radiation reflected by and radiated from the Earth. The instrument operates in a push-broom configuration with a wide swath. Light from the entire swath is recorded simultaneously and dispersed onto two-dimensional imaging detectors: the position along the swath is projected onto one direction of the detectors, and the spectral information for each position is projected on the other direction. From the spectra obtained it is possible to retrieve information on the total column densities and vertical profiles of a number of atmospheric trace gases like NO₂, O₃, CH₄, CO and SO₂. In addition, information relating to clouds, surface reflectance, and aerosols can be derived. The swath is 108 degrees wide and this, combined with a polar circular orbit of 817 km altitude, allows TROPOMI to achieve complete daily surface coverage.

A functional block description of the TROPOMI architecture is given in Figure 1. In the rest of Part II each of the main components of the instrument is briefly described.

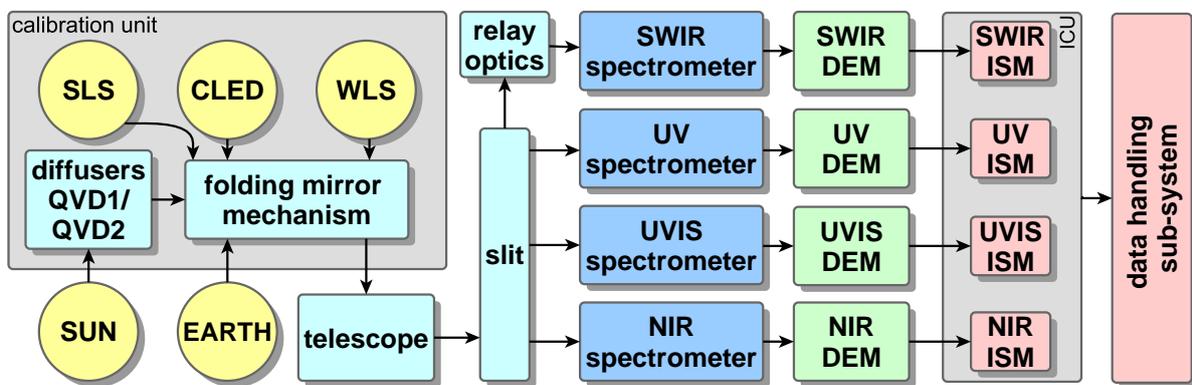


Figure 1: The overall architecture of TROPOMI. Via the calibration unit, light from the Earth, the Sun or from one of the on-board calibration sources (spectral line source (SLS), common LED (CLED) or white light source (WLS)) reaches the detectors. The wavelength bands TROPOMI detects are distributed optically and spatially over the four spectrometers. The signals detected by the spectrometers are digitalized in the detector electronics modules (DEMs). The data is saved and co-added in the instrument specific modules (ISMs) in the instrument control unit (ICU). Eventually the data is transferred to the spacecraft data handling system from where it is transmitted to a ground station.

7 Optics

7.1 Layout

TROPOMI utilizes a single telescope to form an image of the target area onto a rectangular slit that acts as the entrance slit of the spectrometer system. There are four different spectrometers, each with its own optics and detector: mediumwave ultraviolet (UV), longwave ultraviolet combined with visible (UVIS), near infrared (NIR), and shortwave infrared (SWIR). The spectrometers for UV, UVIS and NIR are jointly referred to as UVN. Radiation for the SWIR spectrometer is transferred by an optical relay part in the UVN system from the telescope to an interface position (the pupil stop) for the SWIR spectrometer. This is done because of the more stringent thermal requirements on the SWIR part of the instrument.

Through a calibration unit the telescope receives light from different sources: the Earth, the Sun and three on-board calibration light sources. The calibration light sources are: a spectral line source (SLS), a white light source (SLS) and a common LED (CLED, as opposed to the detector LEDs). Additionally, the calibration unit can act as a shutter (see Section 7.11).

Spectrometer	UV		UVIS		NIR		SWIR	
Band ID	1	2	3	4	5	6	7	8
Performance range [nm]	270–320		320–490		710–775		2305–2385	
Spectral range [nm]	270–300	300–320	320–405	405–500	675–725	725–775	2305–2345	2345–2385
Spectral resolution [nm]	0.5	0.5	0.5	0.5	0.5	0.5	0.23	0.23
Slit width [μm]	560	560	280	280	280	280	308	308
Spectral dispersion [nm/pixel]	0.065	0.065	0.20	0.20	0.124	0.124	0.084	0.097
Spectral magnification	0.327	0.319	0.231	0.231	0.263	0.263	0.025	0.021

Table 1: Main spectral characteristics of the four TROPOMI spectrometers and the definition of the TROPOMI spectral bands with identifiers 1–8.

Each of the detectors is divided in two halves, which yields a total of eight spectral bands. Table 1 summarizes the main characteristics of each of the TROPOMI optical spectrometers and the definition of the spectral bands.

7.2 Telescope

The telescope (see Figure 2) is a two-mirror reflective telecentric telescope that follows an $f-\theta$ law, i.e., it has the property of creating a flat image field at the plane of interest, with a focused beam that is always perpendicular to that plane. It has a large field-of-view in one direction (swath, across track, across flight, or spatial direction), and a small field-of-view in the other (along track, along flight or spectral direction). This is shown at the top and bottom of Figure 3. The two telescope mirrors are referred to as primary and secondary mirror, in the order in which light from the Earth passes through the telescope. A strip on the Earth’s surface is imaged by the first mirror. The intermediate image, located close to the primary, is re-imaged by the secondary on the entrance slit of the spectrometer system. At the same time, the entrance pupil is imaged to infinity. Both mirrors are concave and aspherical. In the optical path between the two mirrors, coincident with the intermediate pupil, there is a polarization scrambler preceded by a rectangular aperture. The latter determines the telescope’s throughput.

The telescope has different f-numbers in the along- and across-track directions. This has been achieved by dimensioning the aperture stop (pupil) to a rectangular shape. The focal length in the two directions is also different, and this has been achieved by making the secondary mirror aspherical. The telescope has a large field-of-view (108°) across track and a small field-of-view along track. In the spectral direction the field-of-view is defined by the width of the slit.

The light for the UVIS and NIR spectrometers passes through the slit. Light destined for the UV and the SWIR spectrometers is reflected from the sides of the slit. Both the SWIR and the UV spectrometers include another slit. A consequence of this arrangement is that the UV and the SWIR are not co-registered with the UVIS and the NIR. The light detected in the UV and SWIR originates from another position than the light detected in the UVIS and NIR. The difference in flight time between the two positions is two seconds, which

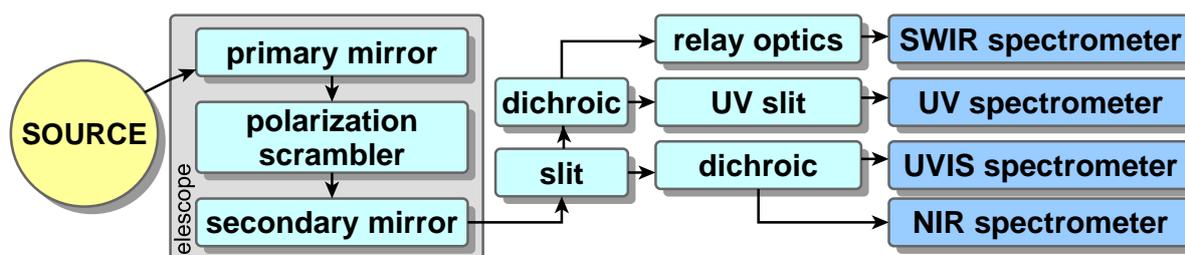


Figure 2: Functional block description of the telescope and the optics distributing the incoming light into the four spectrometers. The slit in the path of the SWIR light is omitted in this schematic.

Spectrometer	UV	UVIS	NIR	SWIR
Telescope entrance area [mm ²]	25	25	25	25
Spatial focal length [mm]	34	34	34	29
Spectral focal length [mm]	68	68	68	29
Spatial slit size [mm]	64	64	64	25.5
Spectral slit size [mm]	0.56	0.28	0.28	0.308
Spatial f-number	<i>F/9</i>	<i>F/9</i>	<i>F/9</i>	<i>F/1.33</i>
Spectral f-number	<i>F/10</i>	<i>F/10</i>	<i>F/10</i>	<i>F/1.33</i>
Spectral IFOV [degrees]	0.48	0.24	0.24	0.25
Spatial sampling distance [degrees]	0.125	0.125	0.125	0.42
Spatial sampling angle along track [degrees]	0.50 [†]	0.50	0.50	0.16
Spatial sampling angle across track [degrees]	0.50	0.50	0.50	0.059

Table 2: Main optical parameters of each TROPOMI spectrometer.

[†]For band 1 the spatial sampling angle is 1.5° and 2.0° in along and across track direction respectively.

corresponds to two read-outs in the baseline configuration. Some of the key geometrical parameters of the instrument are given per spectrometer in Table 2.

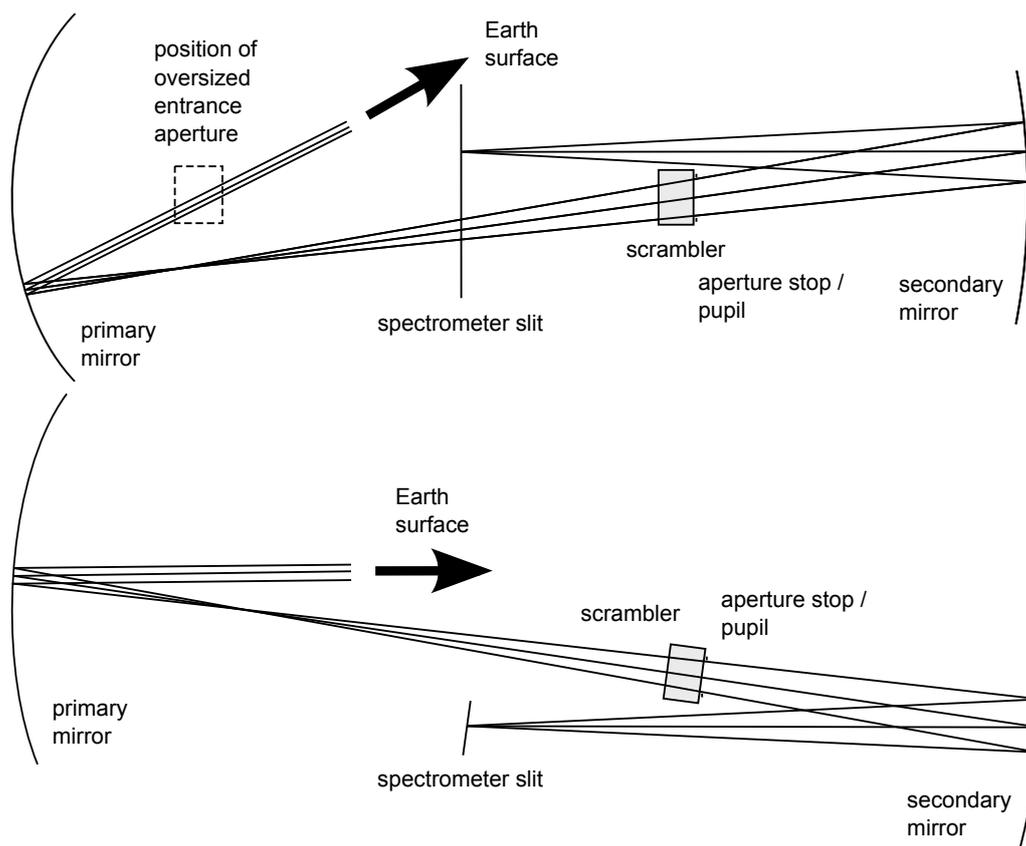


Figure 3: Cross-section of the TROPOMI telescope in the across track (top) and along track (bottom) direction.

Parameter	Wedge 1	Wedge 2	Wedge 3	Wedge 4
Material	MgF ₂	SiO ₂	MgF ₂	SiO ₂
Angle	1.35°	0.6°	1.35°	0.6°
Orientation	90°	-90°	-30°	150°
Crystal axis orientation	90°	0°	45°	135°
Central thickness [mm]	2.0	2.1	2.0	2.1

Table 3: Design values for the wedges of the polarization scrambler. The wedge angle is defined as the angle between the front and the back surface of the wedge. The wedge orientation is defined as the angle between the *x*-axis (flight direction) and the direction of decreasing thickness. The crystal optic axes of all four wedges are perpendicular to the *z*-axis (optical axis; black arrows in Figure 4).

7.3 Polarization scrambler

The polarization scrambler, depicted in Figure 4, is located between the primary and secondary mirrors, and comprises two wedge pairs. The design parameters for the scrambler are summarized in Table 3. The thicknesses are optimized to cancel out the birefringence of each wedge pair along the optical axis. This results in different thicknesses for wedges made out of MgF₂ and SiO₂ respectively, due to the slightly different birefringence of the two materials.

The different optical paths for light with perpendicular polarization due to remaining birefringence causes the so-called diamond effect. The perpendicular polarizations are imaged on slightly different positions on the detector, forming a diamond shape. The calculated values for the diamond effect are shown in Table 4. The minimum and maximum sizes of the diamond, which depend on the wedge angles and on the difference between the ordinary and the extraordinary path, have been calculated over all wavelengths.

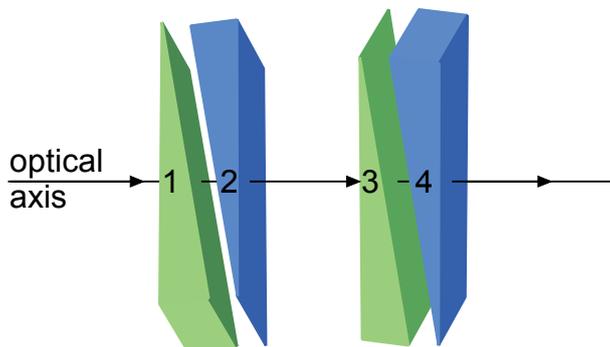


Figure 4: Schematic layout of the polarization scrambler. The scrambler consists of two wedge pairs. The light propagates in the direction indicated by the arrows.

	Minimum (degrees)	Maximum (degrees)
Full width (along track)	4.47×10^{-2}	8.66×10^{-2}
Full width (cross track)	6.13×10^{-2}	7.56×10^{-2}

Table 4: Minimum and maximum values for the diamond effect due to the polarization scrambler.

Spectrometer	UV	UVIS	NIR
Line density [mm^{-1}]	2400	1200	1452.857
Angle of incidence [degrees]	38	45	50
Diffraction order	-1	-1	-1
Efficiency	$\geq 55\%$	$\geq 60\%$ for $\lambda \in [305, 360]$ $\geq 55\%$ for $\lambda \in [360, 550]$	$\geq 45\%$ for $\lambda \in [675, 710]$ $\geq 55\%$ for $\lambda \in [710, 775]$
Performance area [mm^2]	60×58	66×58	58×56
Polarization sensitivity (s/p)	$\in [0.5, 2]$	$\in [0.5, 2]$	$\in [0.4, 2.4]$ for $\lambda \in [675, 710]$ $\in [0.5, 2]$ for $\lambda \in [710, 775]$
Coating	aluminum	aluminum	aluminum/gold

Table 5: Main parameters of the UVN gratings. The physical dimensions of the gratings are a few millimeters larger than the performance area. The UVN gratings are all reflective gratings.

7.4 UVN optical bench module

The three UVN spectrometers are conceptually almost the same: each images a slit on a detector, dispersing the light by means of a grating. The gratings differ per spectrometer; their parameters are listed in Table 5. The diffraction angles for the UVN spectrometers are depicted in Figure 5. The UVIS and NIR spectrometers

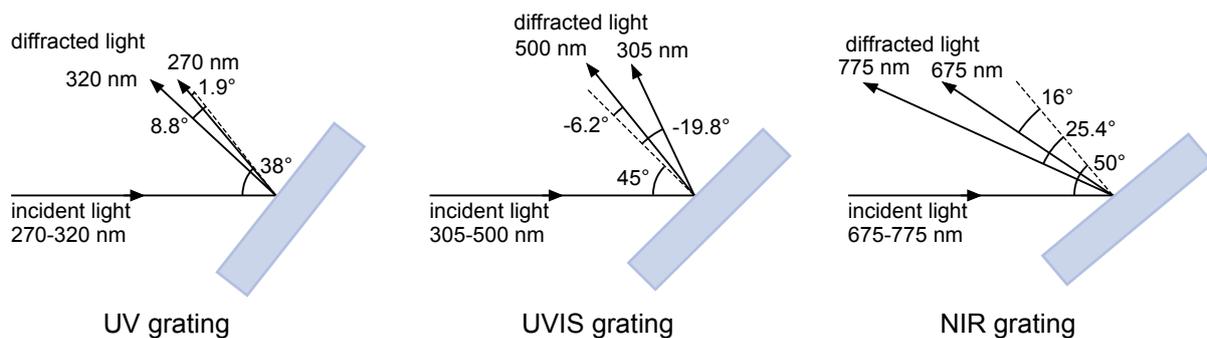


Figure 5: Details of the gratings for the UVN spectrometers. The gratings are a few millimeters larger than the performance area listed in Table 5.

share the same $280 \mu\text{m}$ -wide slit as shown in Figure 6. Light for the UV and SWIR spectrometers first reflects off the UVIS-NIR slit and then, after passing through a dichroic that directs the shortwave component of the light towards the SWIR relay optics, is imaged on a second slit on a conjugate plane to the focal plane of the telescope. This slit is $696 \mu\text{m}$ wide on its conjugate plane, which corresponds to a virtual slit with a width of $560 \mu\text{m}$. Using cylindrical optics, the slit is imaged only in the spectral dimension. This removes the strict requirement on the sharpness of the slit edges in the spatial dimension.

At the end of the spectrometer, the light falls onto a charge coupled device (CCD). One direction of the CCD corresponds to the spatial (across track) dimension, the other direction corresponds to the spectral (along track or flight) dimension. The CCD pixel size is $26 \mu\text{m} \times 26 \mu\text{m}$, and the total number of pixels in the imaging area is 1024×1024 . The image of the slit in the across track direction is about 862 pixels wide, the remaining pixels being used for calibration and monitoring purposes. The dimensions of the slit image on the detector are

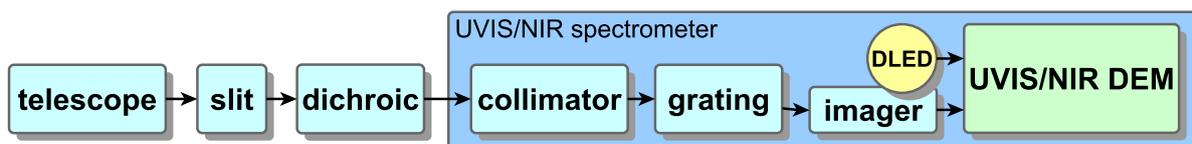


Figure 6: Schematic of the UVIS and the NIR spectrographs. Both the light in the UVIS and the NIR range passes through the slit.

Spectrometer	UV	UVIS	NIR
Full range [pixels], smile excluded	770 × 862	944 × 862	527 × 862
Full range [pixels], smile included	778 × 862	958 × 862	551 × 862
Performance range [pixels], smile excluded	770 × 862	867 × 862	527 × 862
Performance range [pixels], smile included	778 × 862	882 × 862	551 × 862

Table 6: Dimensions of the slit as imaged on the CCDs of the UVN spectrometers.

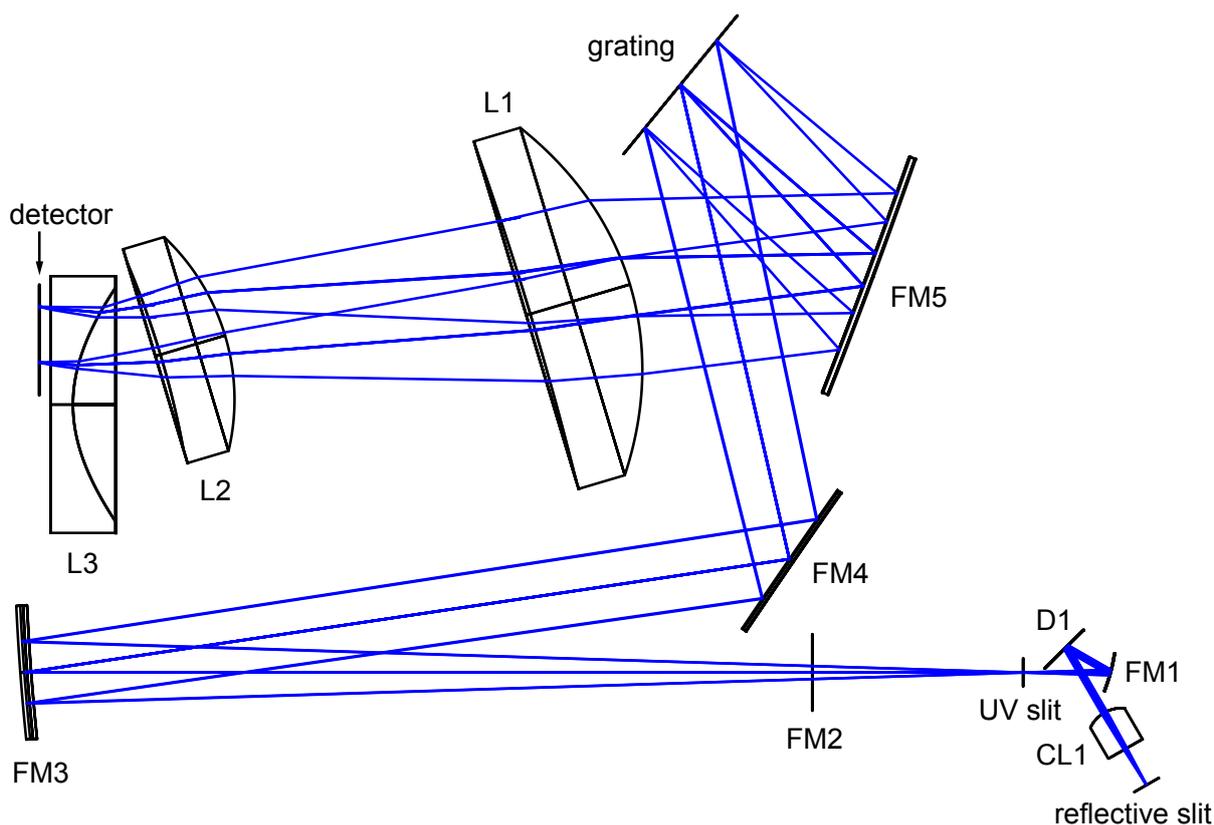


Figure 7: Optical layout of the UV (270–320 nm) spectrometer. The UV light is reflected off the slit, collimated by a lens (CL1) and reflected by a dichroic (D1) and a mirror (FM1) onto the UV slit. Via folding mirrors (FM2–5) the light is guided to the grating. The diffracted light is imaged by a system of lenses (L1–L3) onto the UV detector.

summarized in Table 6. During data acquisition, pixels can be binned in the spatial direction to decrease noise at the cost of resolution (see Section 9 for details).

7.5 UV spectrometer

The optical layout of the UV spectrometer is shown in Figure 7. The view shown is the spectral direction, the telescope is not shown. The beam from the telescope is imaged on the slit telecentrically, as mentioned above. Light for the UV spectrometer actually reflects off the slit, therefore this first slit is not yet the limiting slit for the spectrometer. The reflected image is re-imaged by use of the optics CL1 and FM1 to the actual entrance slit (UV slit) of the spectrometer. The dichroic shown separates the SWIR band from the UV band. The element FM2 is an out-of-plane folding mirror, not incorporated in this view for clarity. Folding mirrors guide the light onto the grating. The diffracted light passes through the imaging optics. The imaging optics consist of three lenses, all three de-centered and tilted with respect to the optical axis in order to get a good co-registration performance and to remove unwanted specular reflections ('ghosts') from the system. The last lens and the CCD plane are tilted, in order to correct for axial color aberrations. To reduce the amount of spectral straylight

that could reach the detector, a spatially varying coating is used on the flat side of L3. At each location on the lens the coating transmits light of the expected wavelength, and it reflects light whose wavelength is 15 nm larger. The geometry of the UV grating is shown in the left part of Figure 5, and its properties are summarized in Table 5.

7.6 UVIS spectrometer

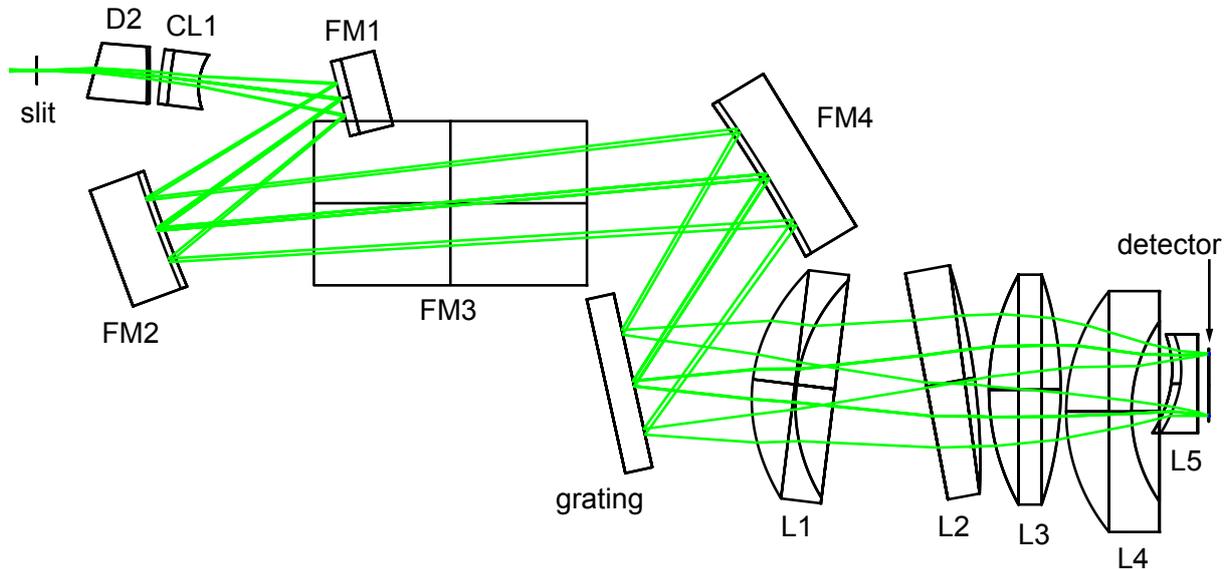


Figure 8: Optical layout of the UVIS (320–490 nm) spectrometer. The UVIS light passes the slit, a dichroic (D2) and collimation optics (CL1). Via folding mirrors (FM1–4) the light is guided to the grating. The diffracted light is then imaged by a system of lenses (L1–L5) onto the UVIS detector.

The optical layout of the UVIS spectrometer is shown in Figure 8. The telescope image is formed on the slit shown in the top left corner in the figure. The light is collimated after passing through a dichroic. Via folding mirrors the light is guided to the grating. Just as in the UV spectrometer, there is an out-of-plane folding mirror (FM3). The grating disperses the light, and the subsequent imaging system images the slit on the detector. The imager consists of five lenses, the last one (L5) having a flat side towards the detector. The geometry of the UVIS grating is shown in the middle in Figure 5, and its properties are summarized in Table 5.

7.7 NIR spectrometer

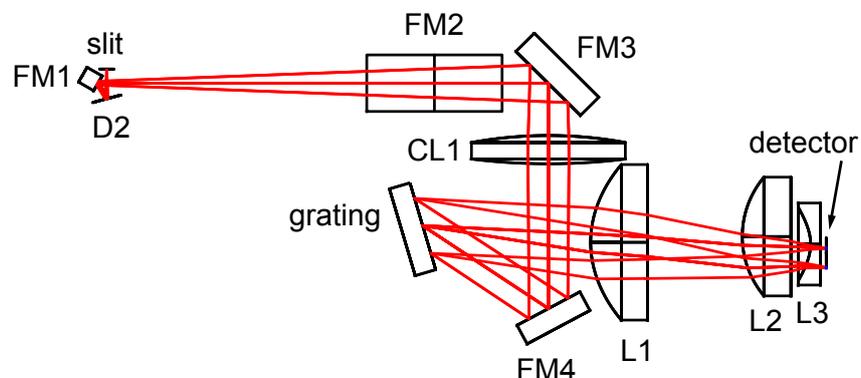


Figure 9: Optical layout of the NIR (675–775 nm) spectrometer. The NIR light passes the slit, is reflected by a dichroic (D2) and transferred via folding mirrors (FM1–4) and collimation optics (CL1) to the grating. The diffracted light is then imaged by a system of lenses (L1–L3) onto the NIR detector.

The optical layout of the NIR spectrometer is shown in Figure 9. The telescope forms an image on the slit, shown in the top left corner of the figure. Via a dichroic (D2) and folding mirrors (FM1–3) and a collimator lens (CL1), the light is guided onto the grating. The dispersed light is imaged on the detector by three de-centered lenses. The geometry of the NIR grating is shown in on the right hand side of Figure 5, and its properties are summarized in Table 5.

7.8 Detector LED

Each UVN spectrometer contains LEDs to illuminate the detectors directly. These detector LEDs (DLEDs) are used for calibration and performance monitoring purposes. The DLEDs emit green light with a wavelength of 570 nm. The response of the individual UVN detectors to the DLED is not identical, as the optical coatings differ per spectrometer.

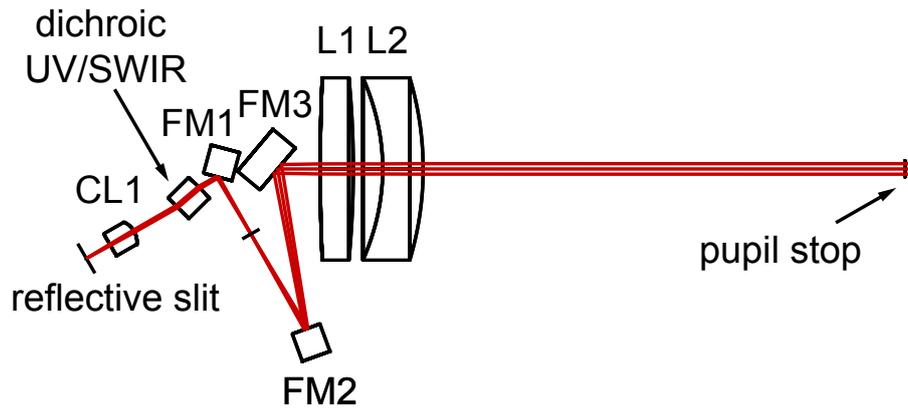


Figure 10: Optical layout of the SWIR relay optics in flight direction. In the across-track direction the beams intersect at the pupil stop with a full angle of 12.68 degrees.

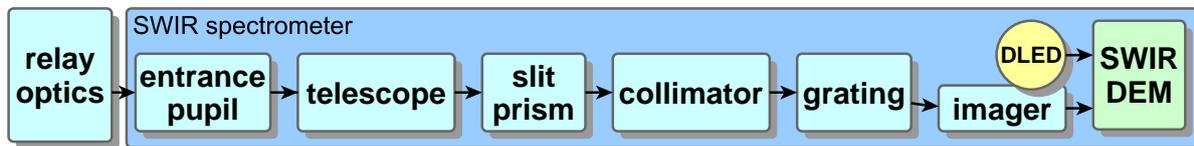


Figure 11: Functional block description of the SWIR spectrometer. The detector LED (DLED) is positioned inside the imaging system.

7.9 SWIR relay optics

The optical layout of the SWIR relay optics is shown in Figure 10. The relay optics are necessary to be able to thermally separate the SWIR spectrometer from the UVN spectrometers. The light from the telescope is imaged onto a pupil at the entrance of the SWIR spectrometer.

The reflective slit, the collimator CL1, and the front surface of the dichroic are shared with the UV spectrometer. The dichroic is made of silicon, providing a good filter function for a wide range of wavelengths. The pupil stop of $9 \times 18 \text{ mm}^2$ is at the end of the relay optics. This stop deliberately vignettes the beam, as this is the stop for the SWIR spectrometer. There is some amount of chromatic aberration, leading to a small magnification error of 0.008%.

7.10 SWIR optical bench module

Functionally, the SWIR spectrometer is similar to the UVN spectrometers (Figure 11). Its optical layout is shown in Figure 12, and a cross section of the entire spectrometer is shown in Figure 13. The optical system is divided into six sections: SWIR entrance pupil, telescope, slit prism, collimator, immersed grating, and imager. The imager interfaces with the focal plane array within the detector module.

The SWIR entrance pupil is formed by the UVN telescope and SWIR relay optics, and it forms the optical interface between the UVN and SWIR subsystems. The SWIR telescope receives its input from the main UVN optics and focuses it on a slit prism. The slit delimits the spatial extent of the image, defining the along track field-of-view, as well as the spectral resolution (in combination with the collimator and the immersed grating). The collimator then transfers the image of the slit to an immersed grating that causes spectral separation. A final imager forms an image of the scene on the SWIR detector.

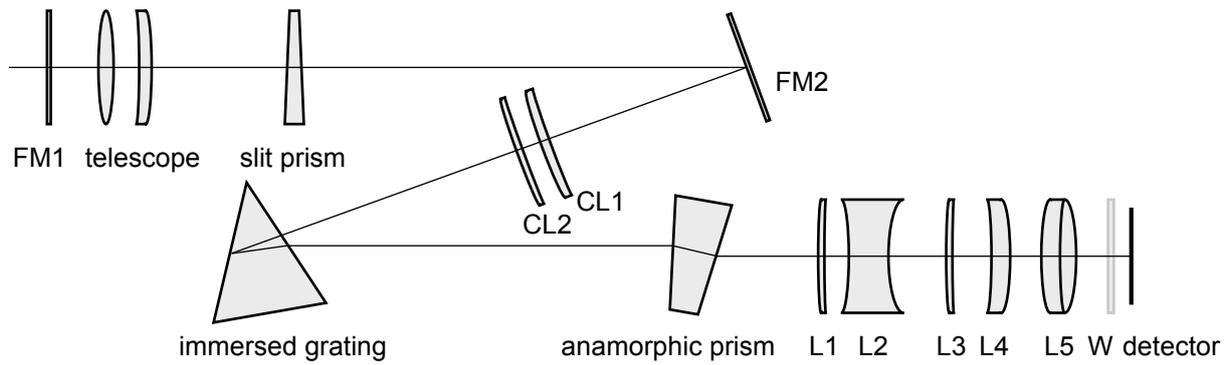


Figure 12: Optical layout of the SWIR spectrometer. The light entering the SWIR spectrometer is guided by the folding mirror FM1 through the telescope onto the slit prism. Via another mirror (FM2) and a collimator (CL1 and CL2) the light reaches the immersed grating. The diffracted beam is re-shaped by the amorphic prism and imaged onto the detector by the lenses L1–L5. A window (W) decouples the detector unit from the optical bench.

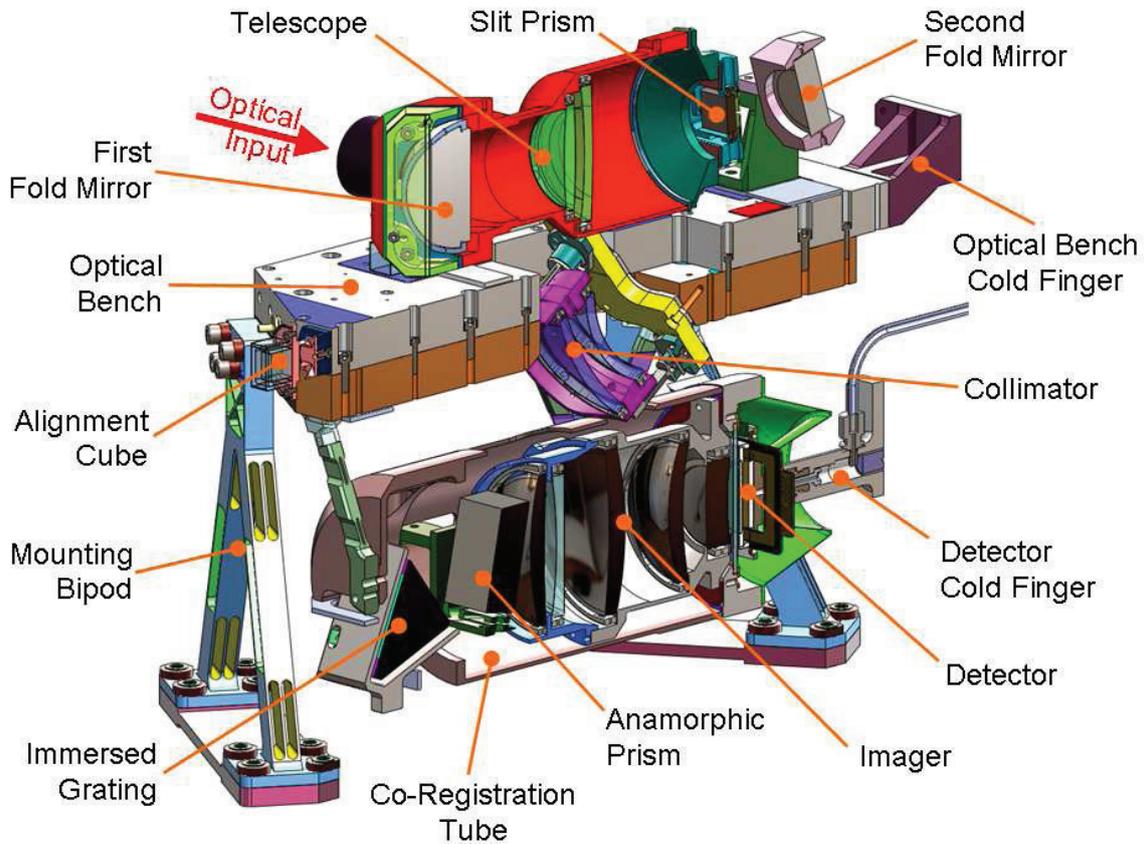


Figure 13: Cut through the SWIR spectrometer. The relay optics are not shown in this schematic.

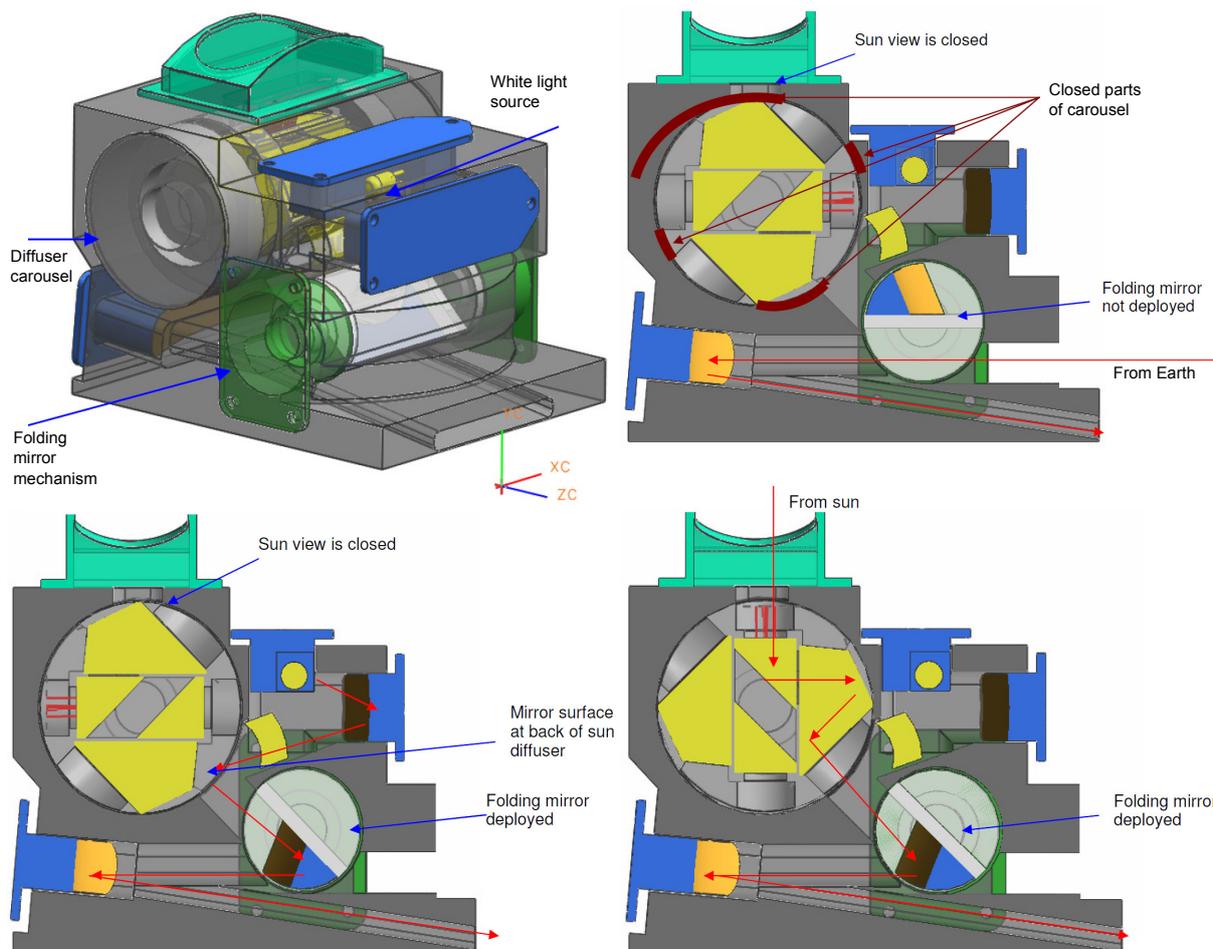


Figure 14: The UVN calibration unit. The folding mirror mechanism reflects the light coming from the calibration unit on the telescope. The diffuser carousel can be set to different positions to guide light from the Sun or the on-board calibration sources (SLS, WLS, CLED) to the folding mirror mechanism. Top left: The calibration unit in overview. Top right: A cut through the closed unit, the telescope views the Earth. Bottom left: A cut through the calibration unit when performing a calibration with the white light source. When the light source is turned off, this configuration can be used to perform dark current measurements. Bottom right: A cut through the unit in the Sun calibration configuration, light from the Sun reaches the primary telescope mirror through one of the two diffusers. The positions of the diffuser carousel for the SLS and the CLED measurements are not shown in these figures.

7.11 Calibration unit

The calibration unit is shown in Figure 14, and its functional decomposition can be seen in Figure 1. It contains two rotation mechanisms: one diffuser carousel and one folding mirror.

The diffuser carousel has six defined positions: one positions for each of the two Sun diffusers, one position for the white light source, one position for the spectral line source (SLS, laser diodes) and two positions for the common LED (CLED). When the diffuser carousel is in the white light source position, the calibration port towards the Sun is closed, so that when the white light source is switched off, a dark measurement can be performed. One of the two Sun diffusers is used to monitor optical degradation and is only employed occasionally for Sun measurements during operation.

The second rotation mechanism deploys a folding mirror in front of the telescope. This folding mirror directs the light from the Sun or the calibration sources towards the primary mirror of the telescope. The folding mirror is curved such that the large field-of-view of the telescope can be completely illuminated. When the folding mirror is deployed, the nadir view is blocked. This means that this mechanism can also function as an instrument shutter.

In the closed position (top right panel in Figure 14), the diffuser carousel is rotated so that the Sun port is

blocked. The closed areas of the carousel are indicated. In this mode the telescope looks directly to Earth. When performing a Sun calibration (bottom left panel), the diffuser carousel is rotated such that it opens the Sun port and directs the light towards the deployed folding mirror. The folding mirror itself closes the nadir port. In the monitoring diffuser mode, the carousel is rotated by 180 degrees with respect to the other diffuser mode. Finally (bottom right panel), calibration with one of the calibration sources (the white light source) is shown. In this case the diffuser carousel is placed in the same position as when closed. The difference is that the folding mirror is deployed so that the telescope receives light from the calibration source. A curved mirror on the back of the Sun diffuser reflects light from the white light source towards the folding mirror. The monitoring diffuser has a flat diffusing surface to reflect the light from the spectral light source towards the telescope.

8 Instrument control unit

The instrument control unit (ICU) is a unit consisting of eight boards with software running on a LEON processor. The main interfaces to the satellite platform are Mil-Bus for command and control and, SpaceWire for science data output.

The ICU hardware includes the following parts: the processing function for the SpaceWire bus; on-board time, synchronization, and clock functionality; image processing and packetization, implemented in one FPGA per DEM; an ICU interface to the four DEMs; thermal control hardware drivers; and a power supply providing ICU internal power and secondary power to the DEMs. The ICU hardware is fully redundant except for the DEM interfaces and image processing, which are implemented as one non-redundant block per detector. The ICU is powered using two redundant power lines.

The ICU software performs the following main tasks: command and control, including command reception, scheduling and execution; parameter management; thermal control; internal and external data acquisition and generation of house-keeping and engineering data packets; science data management; and on-board time synchronization control.

The ICU is equipped with four identical, instrument specific modules (ISM), each controlling one DEM. For the three UVN-DEMs, the ICU controls the details of each frame transfer, line transfer, and line read out. In the case of the SWIR-DEM, the ICU only provides a signal to start the image acquisition, the details being left to the SWIR-DEM itself. For the UVN CCD detectors, each detector is split into two halves as dictated by the detector design and illustrated in Figure 20. This corresponds with the two bands per CCD detector as listed in Table 1. For consistency, the SWIR CMOS detector/spectral range is divided into two halves/bands as well.

The received pixel data arrives row by row, i.e. all pixels of the first row are received first, followed by all pixels of the next row, and so on. Depending on the binning scheme used (applicable to UVN only), a read-out of an entire exposure might consist of any number of rows from 0 to 1024 for each detector half. Image processing in the ICU is performed independently for the halves of a detector.

Up to 800 pixels (columns) can be read out from each detector half. The same number of pixels must be read from each half on one DEM. The co-addition factor can be set to be between 0 and 512, and it can be programmed for each half. It is possible to co-add up to 256 consecutive images.

Information concerning the individual signals of a pixel that contribute (i.e. add up to) to a co-addition is lost, with one exception. One configurable detector pixel, in every row, for both detector output chains, i.e., two columns per detector, is also stored separately for every exposure/co-addition of an image. The data for these 'small-pixel columns' are included in the science data and provide information on a higher spatial resolution than the data for other columns, which may be useful for certain studies.

8.1 Instrument exposure synchronization

Instrument synchronization is accomplished by defining the timing of the Frame Transfers (FTs) for the detectors.

Table 7 gives an overview of all parameters used defining the FTs for the detectors.

Figure 15 depicts an example of the relation between the parameters. The start of a 'Master cycle period' (MCP) triggers an FT after a delay of 'FT sequence offset'. The ISM will generate an FT after a duration of 'FT sequence period'. The first FT of a new MCP must occur one 'FT sequence period' after the last FT in the previous MCP. This results in the constraint that the MCP should be an integer multiple of the FT sequence period. This multiplier is defined in the 'FT sequence count' parameter: 'FT sequence count' * 'FT sequence period' = 'Master cycle period'.

Each FT sequence contains a detector exposure and a readout. A description how the detectors implement an FT sequence can be found in the sections 9.1.5 and 9.2.4. The ISM can co-add the output of several reads in a single measurement. This is specified using the 'Co-addition factor' parameter. The number of (co-added)

Parameter	Level	Description
Master cycle period	Instrument	Duration of the Master cycle period of the instrument
FT sequence offset	Detector	FT sequence offset at the start of a master cycle
FT sequence period	Detector	Duration of a single FT sequence
FT sequence count	Detector	The number of (exposure) frames in an master cycle
Co-addition factor	Band	The number of (exposure) frames co-added to form a single measurement

Table 7: Parameters used for synchronizing the frame transfers between detectors.

measurements in a MCP should be an integer. Therefore the 'FT sequence count' parameter should be an integer multiple of the 'Co-addition factor'.

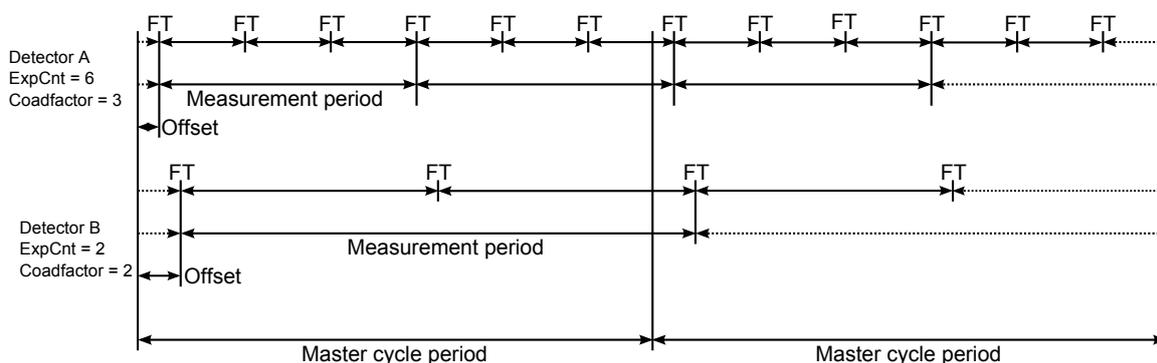


Figure 15: Frame transfer synchronization.

The main synchronization parameter of the instrument is the Master cycle period which is defined on instrument level. All FT sequences are derived from this parameter. Synchronization of the FT sequence between detectors is accomplished with the following assumptions and restrictions.

- All ISM configurations contain the four FT sequence definitions for all detectors for synchronization purposes. The FT sequence can differ per detector.
- The synchronization mechanism prevents readout of frame lines of other detectors during FT.
- The Master clock period is defined as 'FT sequence period' * 'FT sequence count' for all of the FT sequence definitions.
- The 'FT sequence count' for a detector is an integer multiple of the 'Coaddition factor' for both bands on the detector.

9 Detector

The projection of the incoming light onto the detectors differs per spectrometer. In Figure 16, the orientation of the “smile”, the projection of East and West (as seen when on the day-side of the orbit), and the wavelengths are indicated per detector. The combination of the orientation of the spatial axis (East-West direction) and the dispersion axis (direction of increasing wavelength) is individual for all four spectrometers. This is a result of the differing optical paths per spectrometer. The detector modules for UVN and SWIR are described in more detail below.

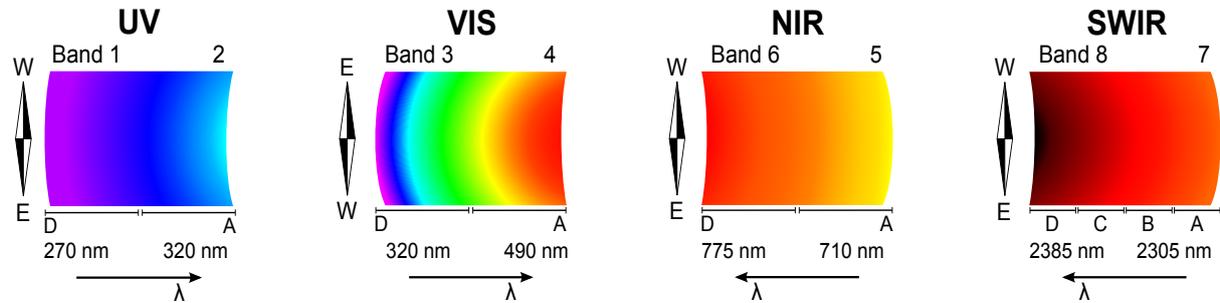


Figure 16: Illustration of the projection of the incoming light onto the four detectors. Indicated are the direction of the “smile”, the projection of East and West and the dispersion direction. The East-West orientation is shown for the day-side of an orbit. The letters label the employed output nodes. The detectors are viewed along the propagation direction of the incoming light.

9.1 UVN detector module

The three UVN spectrometers are equipped with separate but identical detector modules (DEMs) of the same type and configuration (for a functional block description of the module see Figure 17). Each UVN-DEM is equipped with a CCD sensor and front-end electronics, providing the raw digitized measurement data to the instrument control unit.

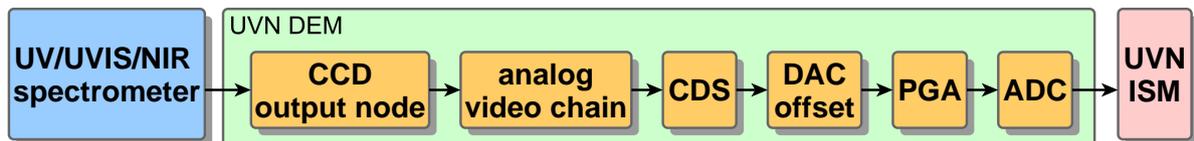


Figure 17: Functional block description of the UVN-DEM.

9.1.1 Mechanical layout

An exploded view of the UVN-DEM is given in Figure 18. The main structure of the UVN-DEM is the detector-side housing which is an aluminum frame. It is the interface to the optical bench on the outside of the UVN-DEM. At the same time, support for the focal plane assembly, including the detector circuit and the thermal bus unit (TBU) side housing, are mounted onto it. The walls near the CCD are designed with an increased thickness in order to maximize radiation shielding. The focal plane assembly consists of the detector circuit including detector, the heat sink, the detector mount and the thermal strap. Its functions are to provide mechanical, thermal, and electrical connections between the detector and the respective interfaces. The TBU-side housing acts as the closing lid of the UVN-DEM and is also the mechanical interface for the main circuit card and for the thermal strap. At the same time it is the thermal interface to the warm TBU stage.

9.1.2 Thermal design

One of the main difficulties of the UVN-DEM thermal design is that the CCD has to remain at a much colder temperature than the electronics boards, which are in the same housing. This creates temperature gradients and the main task of the thermal design is to control these gradients so that both CCD and electronics can

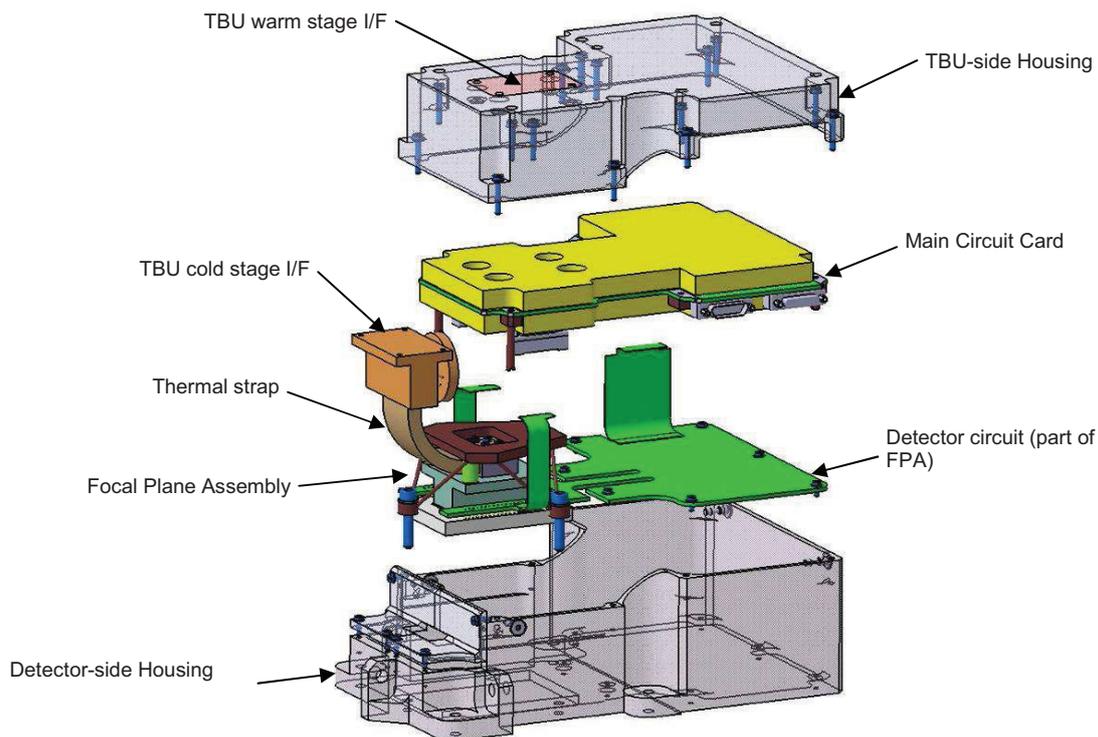


Figure 18: Exploded view of the UVN-DEM.

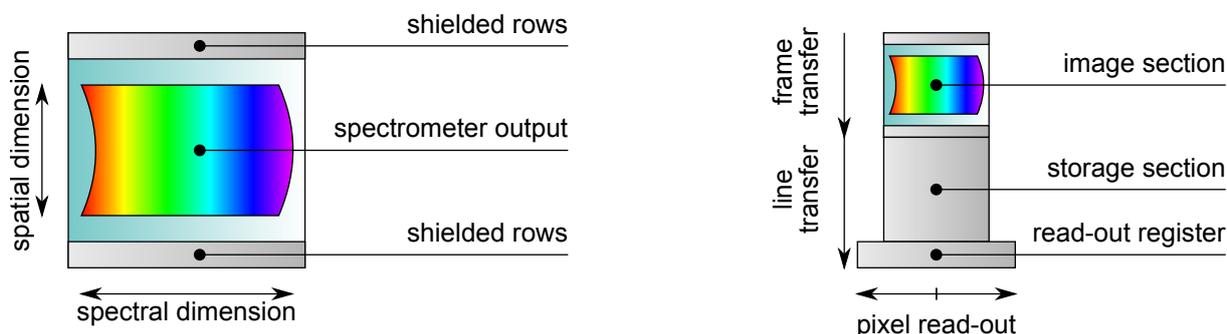


Figure 19: Layout of the UVN CCD Detectors.

be operated in their own temperature range. Critical to the scientific performance is the insulation of the detector from the electronics because their operating temperatures differ by about 80 K. This is achieved by encapsulating the CCD in a box shaped multi-layer insulation. As the CCD has to be operated at cold temperatures, it is thermally linked to a cold finger interface. Additionally, the detector is mounted on a hexapod whose legs provide the required thermal insulation from the rest of the housing.

9.1.3 Detector and electronics

The detector chosen for the UVN is a CCD275 charge-coupled device (CCD) detector, manufactured by e2v. This is a 2-dimensional, back-illuminated frame-transfer sensor with a split read-out register. The detector layout is shown in Figure 19. The detector consists of an unshielded image section, connected to a shielded storage section in which the pixel charges are (ideally) unaffected by the incoming light, which is in turn connected to the read-out register. Both the image section and the pixels are square, being 1024×1024 pixels and $26 \mu\text{m}$ per side, respectively. The storage section has two additional rows, i.e., 1026 rows in total.

The spectral dimension of the spectrometer output is projected onto the columns of the detector, the spatial dimensions is projected onto the rows of the detector. As shown in the left of Figure 19, the spectrometer output does not illuminate all the pixels of the detectors: Approximately 864 rows of the image section will be

illuminated. The top and bottom 35 rows (approximately) of the image section will be shielded, similar to the storage section. This means that these rows are (ideally) unaffected by the incoming light. Due to the frame transfer, these rows are subject to exposure smear, which means that these rows can be used for monitoring or estimating exposure smear. There are rows in between the shielded rows and the spectrometer output. These rows do not receive light from the spectrometer, but since they are not shielded, they do collect straylight. These rows can thus be used for monitoring or estimating straylight.

The pixels of the image and storage sections and the read-out register are connected into vertical shift chains, i.e., the charges of the pixel cells can be shifted down line by line. A frame transfer is an operation in which 1026 such line shifts are performed in quick succession, moving the contents of the image section into the storage section, shifting in zero-charge lines from the top and shifting the charge of the bottom lines into the read-out register. At the end of the frame transfer, the entire image section, as well as the top-most line of the storage section, are emptied of charge and the old image section contents are moved to the 1024 bottom-most lines of the storage section. After the frame transfer, a new exposure starts in the image section, while the finished exposure is read out from the storage section. The frame transfer operation is handled internally by the UVN-DEM, upon reception of a command to initiate a frame transfer. A two-phase clocking scheme is used to achieve a frame transfer time of $\leq 800 \mu\text{s}$.

Once the frame is transferred to the storage section, the read-out starts. A line transfer is an operation in which only the charge in storage section is shifted down one line, leaving the contents of the image section unaffected. The operation shifts a zero-charge line into the top-most line of the storage section and the charge of the bottom-most line is shifted into the read-out register. The charge shifted into the read-out register is added to the charge already there. The process of shifting multiple lines into the read-out register before it is read out (and thereby emptied) is called binning or row binning. The advantages of row binning are that it decreases the data rate and increases the signal-to-noise ratio. The disadvantage of binning is that resolution (information) is lost, as it is an irreversible process. The row binning factor is not necessarily the same across the CCD, but can be varied through instrument configuration. This allows, for example, to influence the ground pixel size across track or to bin all the rows from shielded rows of the image section into a single row.

Once the charge is shifted into the read-out register, it can be read out by shifting the charge pixel by pixel (column by column) onto the output node(s) of the detector. The TROPOMI UVN CCDs have four output nodes per detector, as illustrated in Figure 20. Only the two outermost output nodes, A and D, are used, effectively dividing each detector into two bands. The read-out register has four pixels on each side in addition to the 1024 pixels (columns) of the image and storage sections of the detector. These pixels, referred to as pre-scan and post-scan pixels can be read out and used for calibration or monitoring purposes. In fact, it is possible to even read past the post-scan pixels; the resulting pixels are referred to as overscan pixels and can be used for calibration or monitoring purposes as well.

The output amplifier, which is connected to the output node, provides two gain settings: these are programmable according to the expected signal strength. The main parameters of the electronic circuitry associated with the sensor are summarized in Table 8. The individual pixels' full-well capacity amounts to about 0.8×10^6 electrons (e^-). After the output node, the signal of each of the detector bands is passed through a video amplifier with a fixed gain and then processed by a National Semiconductor LM98640QML integrated circuit. This circuit contains a correlated double sampling unit (CDS), a unit where a programmable offset can be added (DAC), an 8-bit programmable gain amplifier (PGA) and a 14-bit analog-to-digital converter (ADC). The main characteristics of the LM98640QML integrated circuit are shown in Table 9. Apart from the CDS gain, all values listed in the table can be set per detector band.

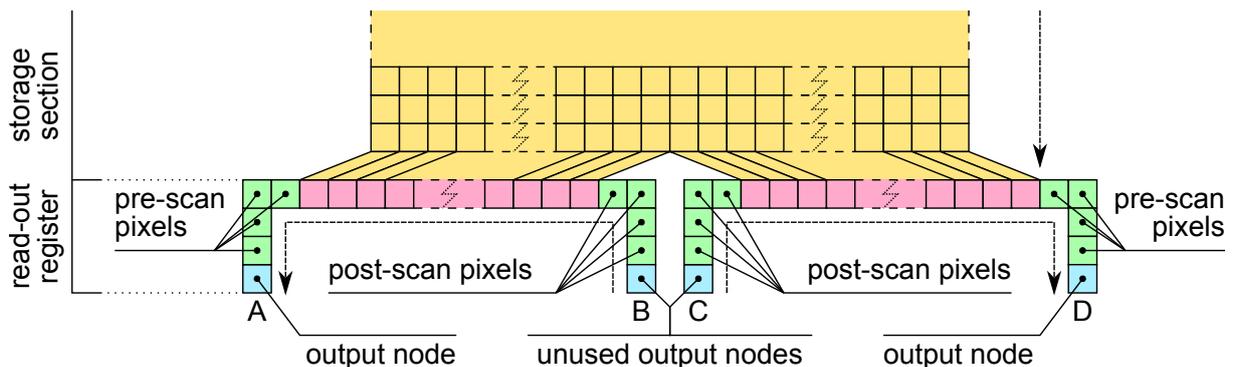


Figure 20: Read-out register of the UVN CCD Detectors.

Spectrometer Band ID	UV		UVIS		NIR	
	1	2	3	4	5	6
Pixel full well [ke^-]	794	810	800	800	817	844
Register full well [Me^-]	3.08	2.82	3.04	3.02	2.95	3.07
CCD gain high [$\mu V/e^-$]	1.46	1.43	1.43	1.47	1.41	1.39
CCD gain low [$\mu V/e^-$]	0.79	0.78	0.79	0.81	0.79	0.79
Analog video amplifier gain	5	1.5	1.6	1.25	1.25	1.4
Read noise rms [LSB] for PGA gain=1, high CCD gain	3.73	2.01	2.07	2.09	2.12	1.93

Table 8: The main characteristics of the UVN detectors and front end electronics.

Parameter	Value
CDS gain	0, 6 dB
DAC offset coarse	± 250 mV
DAC offset coarse stepsize	1 mV
PGA gain steps	256
PGA gain range	-3 dB to 18 dB
ADC resolution	14 bit
read-out noise	2–3.6 LSB

Table 9: The main characteristics of the National Semiconductor LM98640QML integrated circuit with CDS, DAC offset, PGA and ADC. For a CDS gain of 6 dB only half the listed DAC range is available.

9.1.4 UVN storage time

As described in section 9.1.3, the readout of the storage area is started once a frame transfer (FT) is completed. Figure 21 contains a depiction of an example that shows how the storage area is read. The instrument starts reading after a FT. Reading is done one read slot at a time. A read slot has the following behavior:

- It is not possible to read more than one binned line in a read slot.
- The instrument stops reading from the storage area when the number of rows that need to be binned for the next measurement row has been read.
- A read slot can read a maximum number of unbinned rows per read slot. This number is defined in the LTCount setting.
- The duration of a read slot is defined in the setting t_{readslot} .
- Reading of the storage area starts at row 0.

The behavior above leads to the following formula for calculating an estimate of the storage time t_{storage} per binned row r_{img} :

$$t_{\text{storage}}[r_{\text{img}}] = t_{\text{readslot}} \sum_{r=0}^{r_{\text{img}}} \left[\frac{\text{bf}[r]}{\text{LTcount}} \right] \tag{1}$$

Here $\text{bf}[r]$ is the binning factor associated with binned row r .

The formula above assumes no skipped row(s). If skipped rows are present, the time required for reading the skipped row(s) should be taken into account.

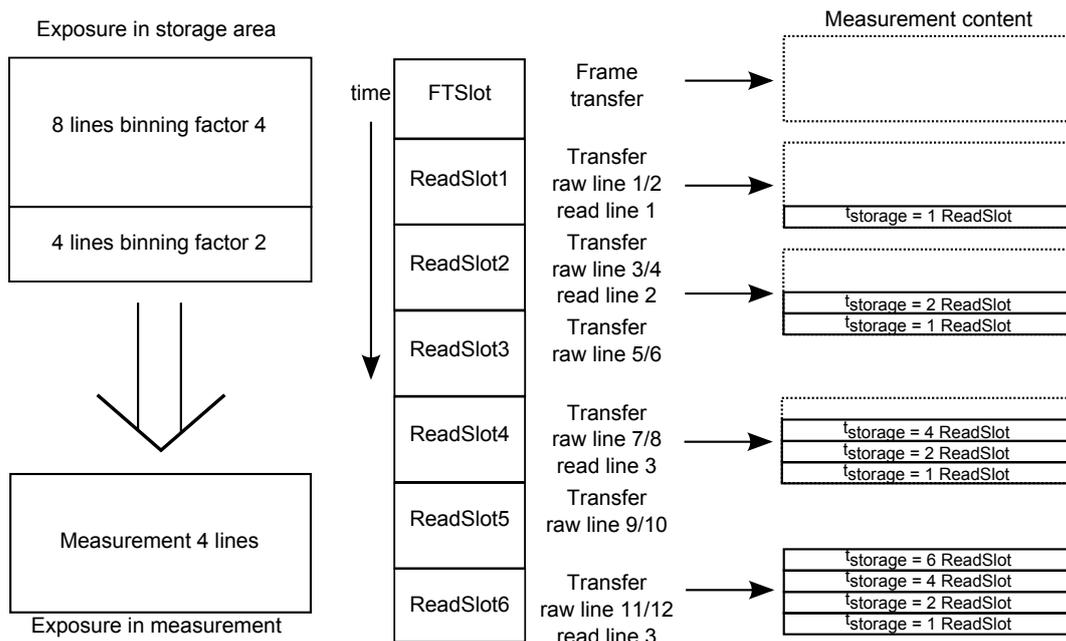


Figure 21: This example shows how 12 detector rows in the storage area are read as image rows in a measurement. The instrument reads a fixed number LTCount of detector rows per read slot (2 in this example). If the number of detector rows to be read is reached, the (binned) value is read into the next line of the measurement. The storage time is therefore an integer multiple of t_{readslot} .

9.1.5 UVN frame transfer sequence

This section contains a description of the frame transfer (FT) sequence of the UVN detectors. The behavior of UVN detectors is characterized using two settings: the ‘Exposure Time’ and the ‘Flush’. These settings are *generic*.

The ‘Exposure Time’ determines the interval between FTs and the ‘Flush’ (n_{flush} , being an integer multiple of the exposure time) is used to suppress FTs after an exposure is finished. The resulting behavior of the UVN detector, as well as the measurement parameters derived from these parameters, are depicted in Figure 22. The list below gives an overview of all parameters in the figure.

- The actual duration of the exposure t_{exp} is defined as the ‘Exposure time’ parameter in the detector settings. Note that this exact relation between value and parameter holds for UVN only.
- The duration of a FT sequence period can be calculated as $(n_{\text{flush}} + 1) \cdot \text{‘Exposure Time’}$. Note that for the SWIR detector, the computation of the FT sequence duration uses the same formula.
- The duration of a measurement can be calculated as ‘FT sequence period’ * ‘Co-addition factor’.
- The time stamp in the L0 measurement data is defined as the time stamp of the FT that triggered the first exposure of the measurement.
- The start time of a measurement (‘MsmtStart’), as defined in the L01b Processor, is defined as the start time stamp of the first exposure in a measurement. This is therefore the same as the time stamp in the L0 measurement data.
- The end time of a measurement (‘MsmtStop’), as defined in the L01b Processor, is defined as the end time stamp of the last exposure in a measurement. It can be calculated as ‘MsmtStart’ + (‘FT sequence period’ * (‘Co-addition factor’ - 1)) + ‘Exposure Time’.
- The measurement time is defined as the mean of the start time of the measurement and the end time of a measurement. It can be calculated as (‘MsmtStart’ + ‘MsmtStop’) / 2.

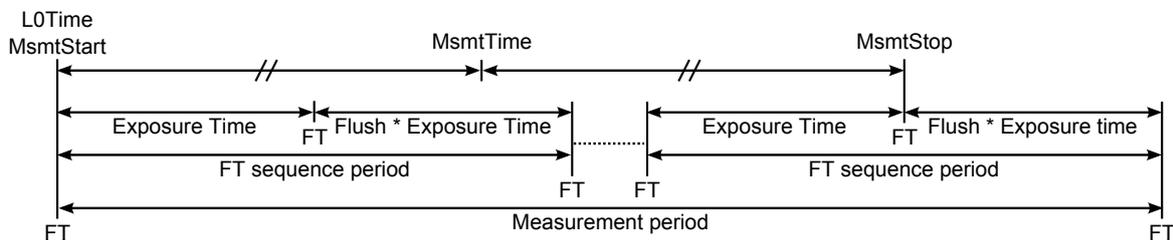


Figure 22: An overview of a FT sequence of an UVN detector.

As explained above, the flush setting can be used to suppress FTs. This is used when the time for reading the storage section is larger than the duration of an exposure. This results in two modes of operation for an UVN detector as depicted in Figure 23.

- In nominal mode, the exposures (frames) are read continuously. Each FT triggers a readout of the storage section: exposure frame $n-1$ is read while frame n is collected in the image section. The instrument is in nominal mode if the ‘flush’ setting is 0.
- In alternate mode, the first FT of a FT sequence triggers an exposure, while the second FT triggers the readout of the storage section. All other FTs in the FT sequence are suppressed. This allows exposure times which are shorter than the readout time of the storage section. The result is a non-continuous readout of exposures. Even though each FT causes a transfer of an exposure to the storage area, the exposure signal that accumulates during the reading of the previous frame is not read and therefore ignored. Since this mode is practical when the read duration of the storage area is longer than the exposure time, the flush is expected to be at least two.

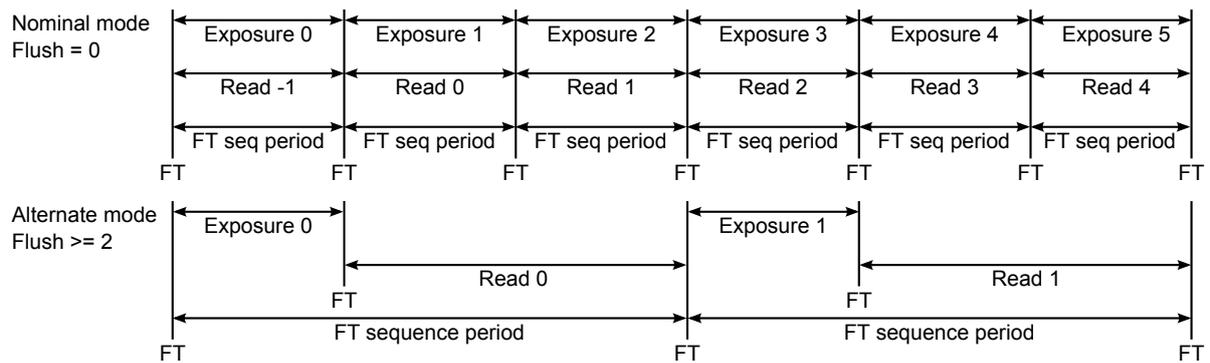


Figure 23: Depiction of the FT sequence in nominal and alternate modes.

9.2 SWIR detector module

A functional block description of the SWIR-DEM is shown in Figure 24. The DEM is equipped with a CMOS detector and front-end electronics providing raw digitized data to the SWIR ISM in the instrument control unit.

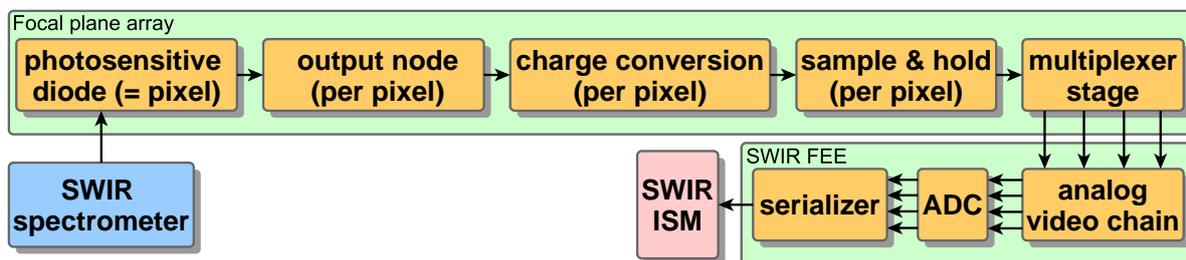


Figure 24: Functional block description of the SWIR detector module and its signal chain. Part of the signal processing is done in the read-out integrated circuit (ROIC) that is part of the focal plane array, and part is done in the SWIR front end electronics (FEE).

9.2.1 Mechanical layout

A cross-section of the mount of the SWIR detector module is shown in Figure 25. An important point for the SWIR detector module is that the temperature of the detector is low and needs to be very stable. To prevent condensation and the forming of ice, a warm window is in front of the cold detector, while venting of the volume is done through the cold finger. The titanium cone provides a stable mechanical suspension with good thermal insulation of the cold detector from the warm spectrometer. The cone is fully closed for electromagnetic interferences (EMI).

9.2.2 Thermal design

The thermal design of the SWIR module aims at keeping the spectrometer, immersed grating, detector, and front-end electronics at the required operational temperatures with sufficient stability. Each component has a different operating temperature, from 140 K (the detector) to 293 K (the front-end electronics). The approach is to overcool the unit as a whole, and then raise and regulate the temperature of each sub-unit through heaters. Although the requirement on temperature stability of the immersed grating is quite strict, analysis has shown that the immersed grating meets the requirement without any dedicated thermal control. This is due to the high thermal inertia of both the SWIR optical bench and the immersed grating and its mount. A temperature sensor on the titanium mount is used for monitoring. The front end electronics reads the two temperature sensors of the detector and controls the temperature of the detector using a PID thermal-control algorithm. Heater power to the detector can be up to 2 W. Achieved temperature stability is about 5 mK rms.

9.2.3 Detector and electronics

The detector chosen for the SWIR is manufactured by Sofradir and of type “SATURN SW”. This is a HgCdTe (or MCT, Mercury Cadmium Telluride) pixel array hybridized on a silicon read-out integrated circuit (ROIC). The detector has 1000 × 256 square pixels (30 μm pitch), and it can be operated in integrate-while-read mode (see Figure 26).

Each pixel is connected to an output stage integrating and amplifying the charges. The charge-to-voltage conversion and sample and hold is done per pixel. The signals of the 1000 columns are multiplexed to four output stages. A schematic of this is depicted in Figure 24. The detector presents four parallel analogue video signals containing sampled detector signals according to the configured read-out scheme. These video signals are buffered and conditioned using low-noise, high-speed video amplifiers that control the offsets, amplitudes and bandwidths. The amplification and conversion takes place in the front-end electronics, and not on the detector. The amplifier adapts the output signal of the detector to fit within the ADC input range. There is margin of 0.5 V on both sides of the ADC range to allow for drifts without the loss of data due to clipping effects of the ADC. The video amplifiers used are LM6172 operational amplifiers. The four video signals are digitized using AD9240 CMOS, 14-bit resolution, 10MSPS ADCs. The main parameters of the electronic circuitry associated with the sensor are summarized in Table 10.

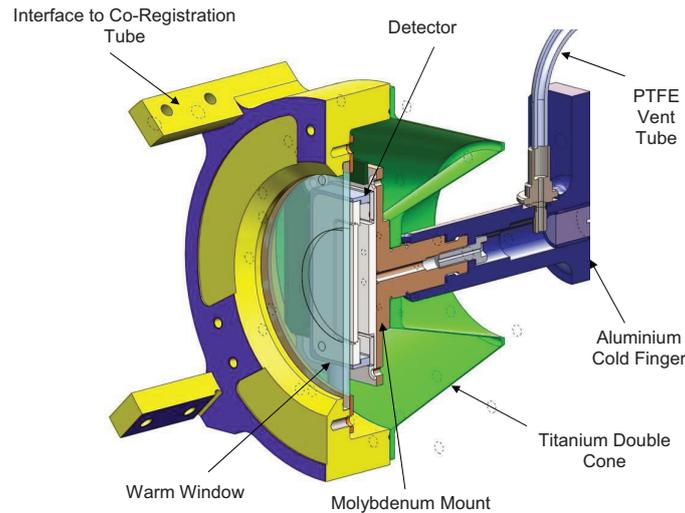


Figure 25: The mount of the SWIR detector. The warm window prevents water-vapor condensation on the cold parts of the detector while the cold finger provides the interface to the cooling system.

Parameter	Value
Pixel full well capacity	$0.5 \times 10^6 e^-$
Read-out noise	$150 e^- r.m.s.$
ADC resolution	14 bit
Effective number of bits	12.6
Dynamic range ADC	6200

Table 10: The main characteristics of the SWIR CMOS detector and its read-out electronics.

A RTAX2000S FPGA carries out all digital control and communications tasks, including detector control, housekeeping and circuit protection, video signal sampling, science data delivery to the ICU and reception/processing of TC/TM signals. The FPGA operates autonomously without an associated processing unit, and is automatically reset every time power is applied. Synchronization is achieved by supplying an external clock oscillator and a periodic timing pulse from the ICU, both via LVDS interfaces. Telecommand and telemetry interfaces will also be provided by way of LVDS links to the FPGA. The FPGA generates all timing and clock signals for the system, including detector clocks, video ADC sampling clocks and communications timing clocks.

9.2.4 SWIR timing

This section contains a description of the FT sequence of the SWIR. The behavior of SWIR is characterized using two generic settings and two SWIR specific settings. The generic settings 'Exposure Time' and 'Flush' determine the FT sequence period, exactly as in the UVN module. The difference is that, after the computation of the FT sequence period, the two generic settings play no role anymore. In particular, the actual SWIR exposure time is not immediately related to the generic 'Exposure Time' setting. Instead, the SWIR specific settings 'IntDelay' and 'IntHold' are used to determine the exposure characteristics. The resulting behavior of the SWIR, as well as the measurement parameters derived from these parameters are depicted in Figure 26. The list below gives an overview of all parameters in the figure.

- The duration of a FT sequence can be calculated as $(n_{flush} + 1) \cdot \text{'Exposure Time'}$, exactly as in UVN.
- The duration of a measurement can be calculated as 'FT sequence period' * 'Co-addition factor'.
- The duration of one SWIR internal Master Clock Cycle (MCC) is $1.25 \mu s$.
- The minimal fixed delay between an FT and an exposure 'Read delay' (RD) is 0.5 MCC ($0.625 \mu s$).
- The programmable extra delay $t_{intdelay}$ before the start of an exposure is set using the 'IntDelay' parameter.

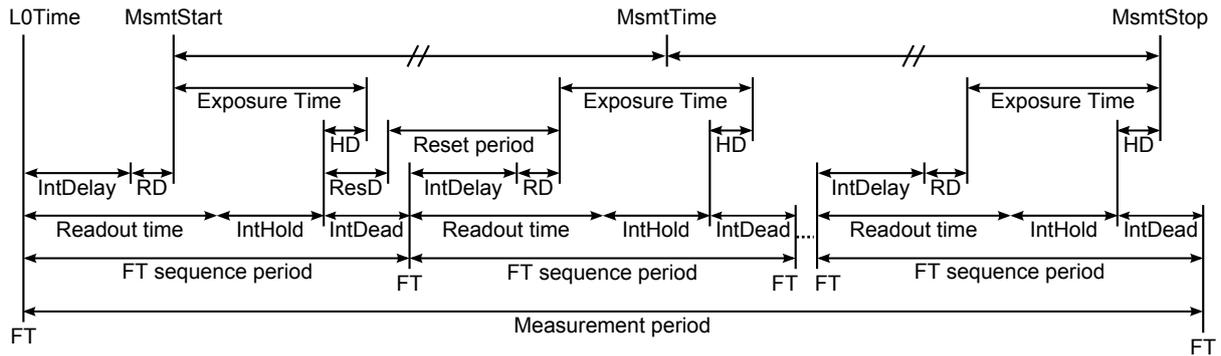


Figure 26: SWIR timing. An overview of the exposure sequence of the SWIR triggered by an FT. The exposure will start after a delay and the FT will also trigger the read of the previous exposure frame.

- The fixed time t_{readout} it takes to read an exposure 'Readout time' is 65536 MCC (81.92ms).
- The fixed delay between the end of a readout and the end of an exposure 'HoldDelay' (HD) is 4.5 MCC (5.625 μs).
- The programmable extra delay t_{inhold} between the end of a readout and the end of an exposure is set using the 'IntHold' setting.
- The time between the end of 'Inthold' and the next FT is called 'IntDead' and can be calculated as 'Intdead' = 'FT sequence period' - 'IntHold' - 'Readout time'.
- The fixed delay before a pixel reset 'Reset delay' (ResD) is 256.5 MCC (320.625 μs).
- The reset of the pixels takes place during the 'Reset period'. During this period the charge on the integration capacitor changes from the previously measured value to zero. 'Reset period' is calculated as 'IntDead' + 'IntDelay' - 'Reset delay' + 'Read Delay'.
- The time stamp in the L0 measurement data is the time stamp of the FT that triggered the first exposure of the measurement.
- The start time of a measurement ('MsmtStart') is defined as the start time stamp of the first exposure in a measurement. It can be calculated as 'LOMsmtTime' + 'Read delay' + 'IntDelay'.
- The 'Exposure time' t_{exp} is the duration of an exposure. It can be calculated as:

$$t_{\text{exp}} = t_{\text{readout}} + t_{\text{inhold}} - t_{\text{intdelay}} + t_{\text{corr}}, \quad (2)$$

where t_{corr} equals 'Hold delay' - 'Read delay', in total 4 MCC.

- The end time of a measurement ('MsmtStop') is defined as the end time stamp of the last exposure in a measurement. It can be calculated as 'MsmtStart' + ('FT sequence period' * ('Co-addition factor' - 1)) + 'Exposure Time'.
- The measurement time is defined as the mean of the start time of the measurement and the end time of a measurement. It can be calculated as ('MsmtStart' + 'MsmtStop') / 2.

For optimal performance, there are constraints on the minimum dead-time and the minimum 'IntHold' time. The dead time following the exposure should last at least 1.5 ms and the inthold time at least 198.75 μs (159 MC). During the dead time the detector is not sensitive to photon flux.

Note that the computed exposure time is assumed to be exact: The engineering parameters 'IntHold' and 'IntDelay' cause no error to t_{inhold} and t_{intdelay} .

10 Straylight performance

Straylight is unwanted light in an optical system and it originates from both intended and unintended light sources. In the case of the former, the straylight follows optical paths that are not intended by the optical design and therefore reaches the detector at unintended positions. This gives rise to spurious signals at the detector.

In this section the different forms of straylight are introduced. Simulations performed for the four spectrometers of the TROPOMI instrument give an indication of straylight levels and paths that straylight takes within the instrument.

10.1 TROPOMI straylight

To illustrate straylight in the context of the TROPOMI instrument, Figure 27 (a) shows the result of a ray tracing simulation at a wavelength of 405 nm for the UVIS spectrometer without straylight. The lenses transmit and the mirrors reflect perfectly and only the rays in the -1^{st} diffraction order of the grating reach the detector. The rays form a spots diagram in a “smile” shape at the detector as shown in Figure 27 (b). This is the expected response of the instrument at a wavelength $\lambda = 405$ nm when neglecting straylight. However, other than this intended light, there are a number of contributions to additional, unintended light on the detector. These contributions are discussed below.

Ghosting In reality lenses and detectors reflect a part of the incoming light as well. Figure 28 (a) shows how a ray that is reflected back from the detector, can undergo another back-reflection at a lens surface and hit the detector at a position completely different from the position intended by the design. The mechanism through which unwanted specular reflections give rise to secondary images on the detector is known as ghosting. The rays following the ghost path illustrated in Figure 28 (a) give rise to the ghost shown in Figure 28 (b). The ghosting effect is a two-dimensional feature, i.e., it extends in both the spectral and the spatial directions of the detector.

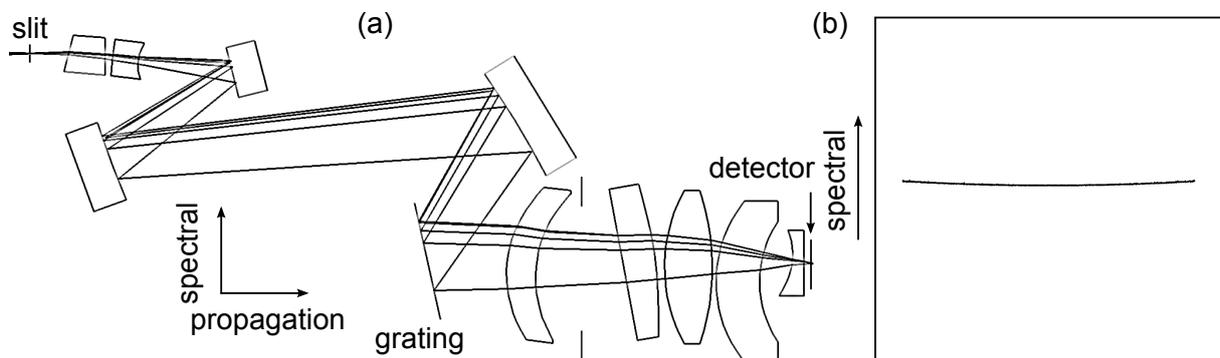


Figure 27: (a) A ray trace for the TROPOMI UVIS spectrometer without straylight at $\lambda = 405$ nm. (b) The corresponding spots diagram at the detector.

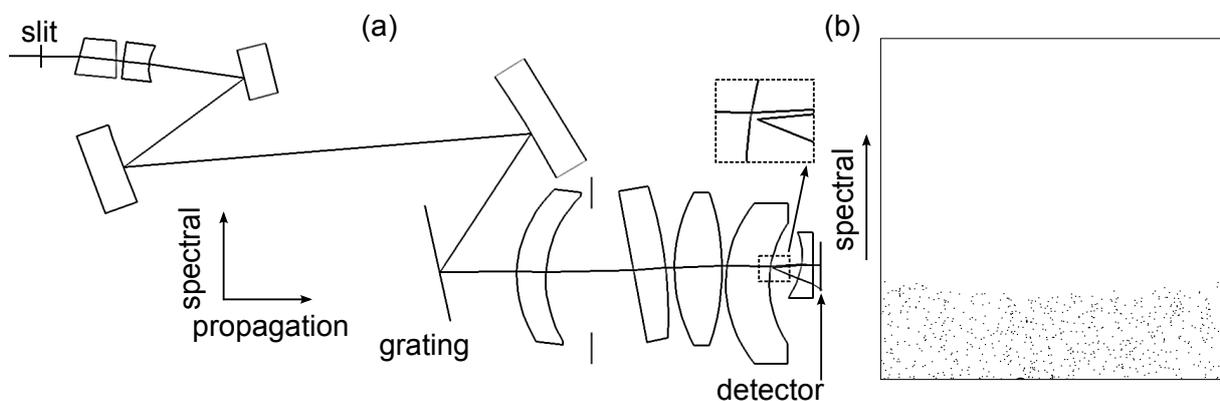


Figure 28: (a) Ghosting in the TROPOMI UVIS spectrometer at $\lambda = 405$ nm. (b) The corresponding spots diagram at the detector.

Scattering In practice, optical surfaces are not perfectly flat and optical media such as optical glasses are not perfectly uniform giving rise to scattering: the change in the propagation direction of light due to localized non-uniformities on the surface and/or in the volume of an optical element. Figure 29 (a) shows how rays scatter due to the surface roughness of the last lens in the UVIS spectrometer. The scattered rays generate the spots diagram shown in Figure 29 (b). Scattering is a two-dimensional effect. The scattering contributions can be divided into two parts: surface roughness and scattering at contamination particles. The former remains constant while the latter is likely to increase after on-ground calibration and therefore the calibration key data will underestimate the straylight occurring in-flight.

Diffraction Light waves diffracting at an obstacle such as an aperture or an opaque edge can also cause straylight. The diffraction effects are most pronounced for wavelengths in the order of the aperture size. For the SWIR spectrometer, operating at wavelengths in the μm range, it is possible that the straylight due to diffraction is non-negligible.

Diffraction grating effects Diffraction gratings introduce additional straylight mechanisms. For example, periodic errors in the groove spacing of a grating introduce unwanted spectral lines called Rowland ghosts. Light in these spurious spectral lines can propagate to the detector contributing to the overall straylight measured by the instrument. Another potential source of straylight caused by diffraction gratings is the light at half the wavelength of the spectrometer spectral range. This light propagates to the detector via the same optical path as the light at the wavelength of the spectrometer spectral range. Light at wavelength $\lambda/2$ in the diffraction order $2m$, has the same optical path as the light at wavelength λ in the diffraction order m . Furthermore, it is also possible that the light reflected back from the detector finds its way back to the detector via the intended diffraction order and/or unintended diffraction orders of the grating. These diffraction grating straylight mechanisms can be considered a special type of ghosting effects.

10.2 Quantitative analysis

To estimate straylight levels in the TROPOMI instrument, optical models of the TROPOMI UV, UVIS, NIR, and SWIR spectrometers have been constructed in a non-sequential ray tracing software package called ASAP (Advanced Systems Analysis Program).

Using these models, the TROPOMI instrument performance has been evaluated with respect to the spatial straylight requirements that are formulated in [RD4]. These requirements are defined for the reference scene shown in Figure 30. For the UVN module, the requirement states that the spatial straylight affecting the spatial samples located in the center of the dark zone (inner part of Figure 30) has to be lower than 5% of L_{dark} assuming that $W = 10$ degrees, $L_{\text{bright}} = L_{\text{max}}$, and $L_{\text{dark}} = L_{\text{ref}}$. Spectral radiances L_{max} and L_{ref} for UVN are shown in Figure 31. For the SWIR spectrometer, the requirement states that the straylight on the spatial samples located in the center of the dark zone (inner part of Figure 30) has to be lower than 4% (threshold) / 2% (goal) of L_{dark} assuming that $W = 15$ SSA (spatial sampling angle) and $L_{\text{bright}} = 10 \times L_{\text{dark}}$. Spectral radiances L_{max} and L_{dark} for the SWIR spectrometer are shown in Figure 32. Figures 33 and 34 show the total spatial straylight in the center of the dark zone as a function of the wavelength bin of the detector for the

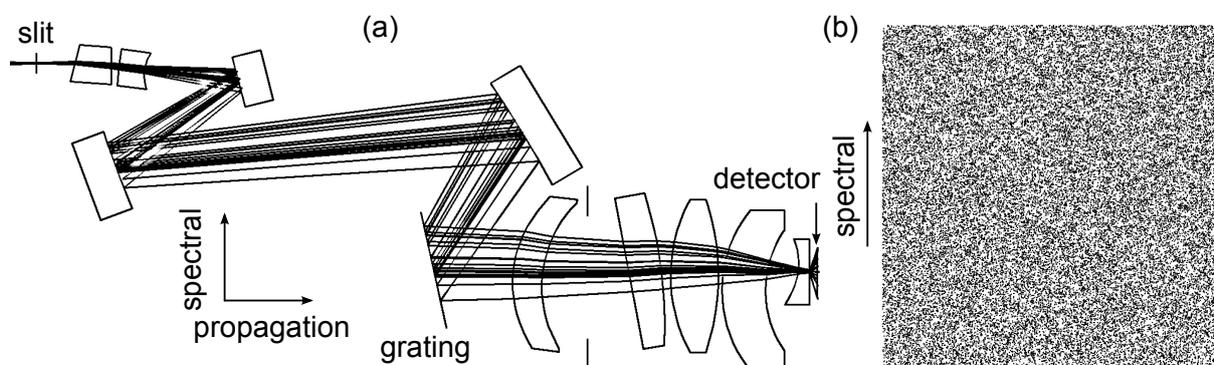


Figure 29: (a) Scattering in the TROPOMI UVIS spectrometer at $\lambda = 405$ nm. (b) The corresponding spots diagram at the detector.

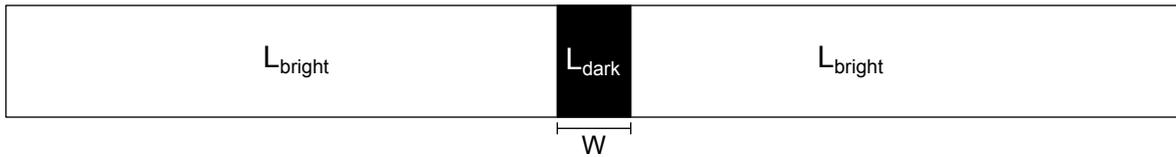


Figure 30: Reference scene for the spatial straylight.

UV and UVIS spectrometers. The total straylight is calculated as the sum of the ghosting and scattering effects. Neither of the three UVN spectrometers is compliant with the spatial straylight requirement.

Figure 33 shows straylight contributions for the UV spectrometer with a graded filter called the modified graded filter. The modified graded filter is a linear variable low-pass filter used to suppress the straylight at longer wavelengths. Namely, for the UV spectral range, the spectral radiance sharply rises from shorter to longer wavelengths (see Figure 31). Consequently, the signal at longer wavelengths gives a large contribution to the straylight at detector region that corresponds to shorter wavelengths. To suppress this straylight, the modified graded filter is placed on the back planar surface of the lens positioned just before the detector. For the UV spectrometer, scattering of the -1st diffraction order from the grating gives the largest contribution to the total scattered power at the detector plane and ghosting is driven by back reflections from the detector followed by back reflections from lens surfaces.

Figure 34 shows straylight contributions for the UVIS spectrometer with the anti-reflection coating at the detector. The anti-reflection coating significantly reduces the strong ghosting effects caused by a 30% reflectance of the bare detector. The strongest ghost path in the UVIS spectrometer is formed by the detector and the grating. The rays in this path reflect from the detector surface back to the grating and via the +1st diffraction order of the grating propagate back to the detector. As in the case of the UV channel, scattering of the -1st diffraction order from the grating gives the largest contribution to the total scattered power at the detector. Figure 35 shows the total spatial straylight (solid black line) in the center of the dark zone as a function of the wavelength bin of the detector for the SWIR spectrometer. In addition to the straylight due to scattering (dotted green line) and ghosting (dotted blue line), the analysis takes into account the straylight due to diffraction (dotted red line) from the entrance pupil of the SWIR spectrometer. Not taking into account the peaks due to the atmosphere absorption lines, SWIR is barely compliant with the spatial straylight requirement.

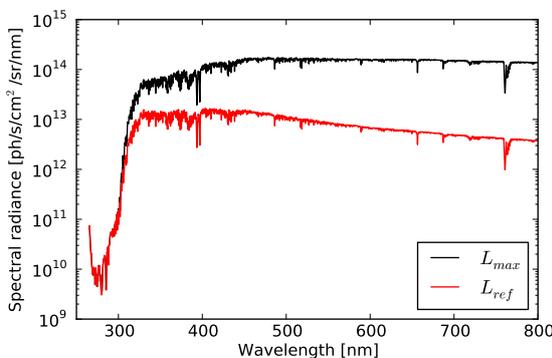


Figure 31: Spectral radiances $L_{max} = L_{bright}$ (black line) and $L_{ref} = L_{dark}$ (red line) for the UVN module.

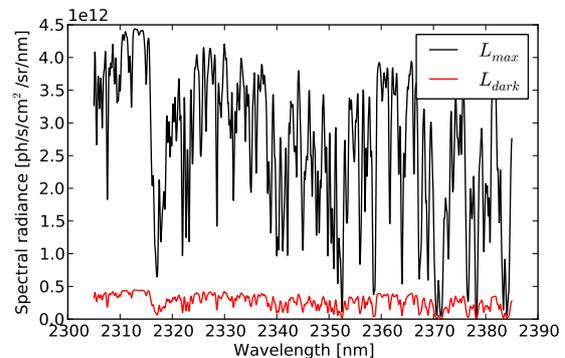


Figure 32: Spectral radiances $L_{max} = 10 \times L_{dark}$ (black line) and L_{dark} (red line) for the SWIR spectrometer.

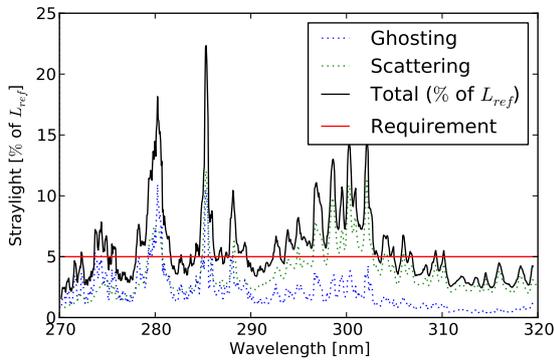


Figure 33: Total spatial straylight in the center of the dark zone for the UV spectrometer with the modified graded filter.

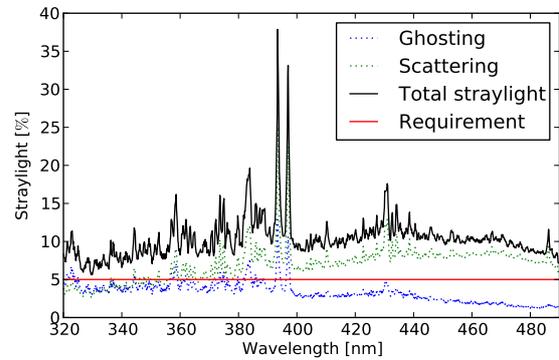


Figure 34: Total spatial straylight in the center of the dark zone for the UVIS spectrometer with the anti-reflection coating at the detector. The straylight is expressed as a percentage of the radiance in the center of the dark zone without ghosting and scattering.

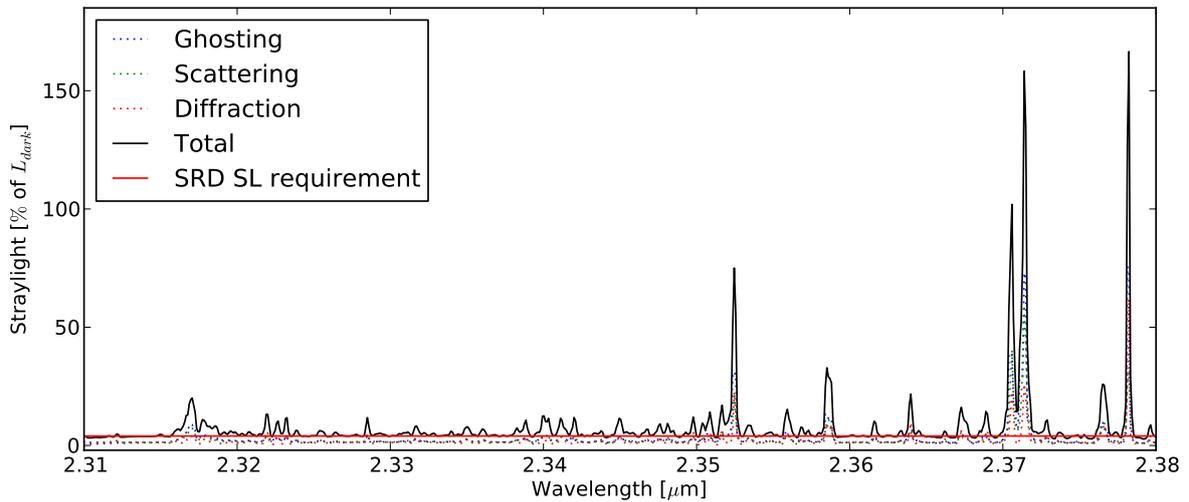


Figure 35: Total spatial straylight in the center of the dark zone as a function of wavelength bin of the detector for the SWIR spectrometer. The straylight is expressed as a percentage of L_{dark} . For the wavelengths of the strong absorption lines straylight poses a severe problem.

Part III

Operational aspects

The TROPOMI Level-1b data products are to a large extent defined by the way that the instrument is operated and the data is processed. This section focuses on such operational aspects and discusses their relation to the Level-1b data products.

11 Orbit definition

The orbit definition of the Sentinel-5p (S5p) mission plays an important role in the operational aspects. Both instrument operations and data processing use a (coordinated) orbital scenario. This orbital scenario is also linked to in-flight calibration of the instrument. Sentinel-5p will fly a sun-synchronous polar orbit, in close formation with NASA's Suomi NPP mission. The orbital parameters for S5p are given in Table 11.

Operational parameter	Value
repeat cycle	17 days
cycle length	241 orbits
semi-major axis	7205.919 km
eccentricity	0.001148 –
inclination	98.7462 deg
argument of perigee	90.00 deg
mean local solar time of ascending node crossing	13:35 hh : mm

Table 11: Reference orbit of the Sentinel-5p mission.

Each S5p orbit has a day (lit) side and a night (dark) side, as illustrated in Figure 36. On the day side the spacecraft flies from south to north; on the night side it flies from north to south. Spacecraft midnight is defined as the time halfway the nadir day-night terminator and the nadir night-day terminator; spacecraft noon is the time halfway the nadir night-day terminator and the nadir day-night terminator. Both the instrument operations as well as data processing will use the spacecraft midnight as the start and end points of an orbit, as further described in Sections 12 and 15. Due to seasonal variation, the position of the equator with respect to the spacecraft midnight will change. As a result, spacecraft midnight is not at a fixed latitude.

12 Instrument operations

For TROPOMI instrument operations, an orbital scheduling approach is used. An orbit is defined from spacecraft midnight to spacecraft midnight, as described in Section 11. Earth radiance measurements will be performed on the day side of the orbit. At the north side of the orbit, near the day-night terminator, the Sun is visible in the instrument's solar port. Approximately once a day, a solar irradiance measurement is performed. The night side of the orbit is used for calibration and background measurements. The following constraints apply to the calibration measurements:

1. Background and calibration measurements can only be performed when the spacecraft is in eclipse.
2. No measurements can be taken around spacecraft midnight, in order to facilitate data processing.
3. All orbits must contain background measurements in the eclipse part of the orbit that match the radiance measurements on the day side for in-flight calibration by the L01b Processor.
4. Calibration measurements must be performed outside the South Atlantic Anomaly (SAA) area, in order to minimize interference of proton radiation.
5. Calibration measurements must have a regular, fixed repetition interval.

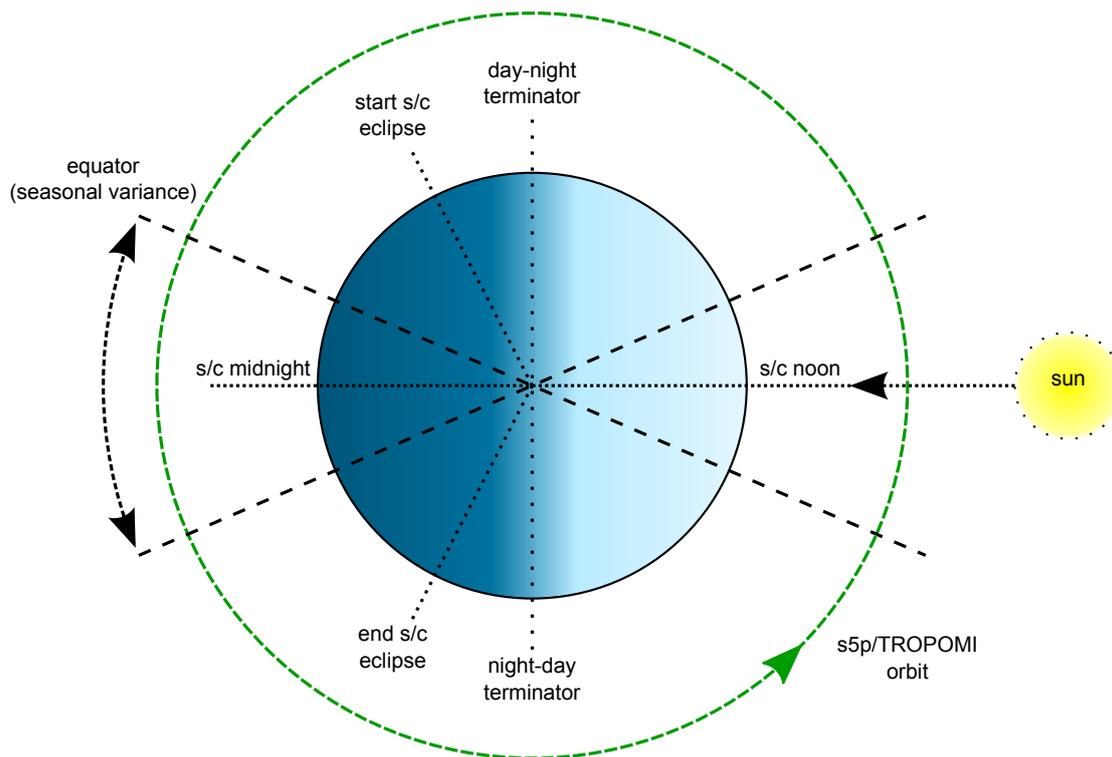


Figure 36: Sentinel-5p orbit overview.

The constraints for the SAA and the spacecraft eclipse greatly reduce the parts of the night side of the orbit that are suitable for calibration measurements. The SAA is bound to a fixed area in terms of latitude and longitude, but due to seasonal variation, its position relative to spacecraft midnight changes over the seasons. This is illustrated in Figure 37, which shows the position of the SAA in the two most extreme situations, i.e. 21 June and 21 December. In Figure 37 the green parts show the part of the orbit that can be used for calibration measurements.

Since for instrument operations, the orbits are defined without any seasonal dependency, only a small part of the orbit is guaranteed to be unaffected by the SAA throughout the seasons. This part of the orbit will be used for calibration measurements, while the remainder of the orbit where the spacecraft is in eclipse will be used for background measurements. This is shown in Figure 38. These background measurements are susceptible for proton radiation too, but the L01b Processor will use a filter to avoid background measurements taken in the SAA being used for in-orbit calibration.

To accommodate regular, fixed repetition intervals for the calibration measurements, a scheme of 360 orbits is used. As 360 is divisible by many numbers, it is possible to accommodate many different repetition intervals. For sake of simplicity, the 360 orbits are divided in 24 blocks of 15 orbits, each block corresponding to approximately 25 hours, or roughly to a day. A 'week' is defined to be 6 of these 15-orbit blocks and a 'month' as 4 of these weeks. This allows for easy definition of calibration measurements that have (roughly) daily, weekly, biweekly or monthly repetition cycles. This is illustrated in Figure 39. The basis is formed by the *orbital* orbits, which contain only Earth radiance and background measurements. The *orbital* orbits are adjusted by adding calibration measurements to create special calibration orbits, depending on the required repeat cycle, *daily*, *weekly*, *biweekly* and *monthly*.

13 Instrument modes

13.1 Instrument configuration

The TROPOMI instrument has many configurable parameters. For example, the exposure time, co-addition period, gains and (for UVN-DEMs) the binning factors can be varied. As a result the instrument can be operated in many different modes or configurations. Each combination of instrument settings is referred to as **instrument configuration** and is identified by an **instrument configuration ID**, a number in the range

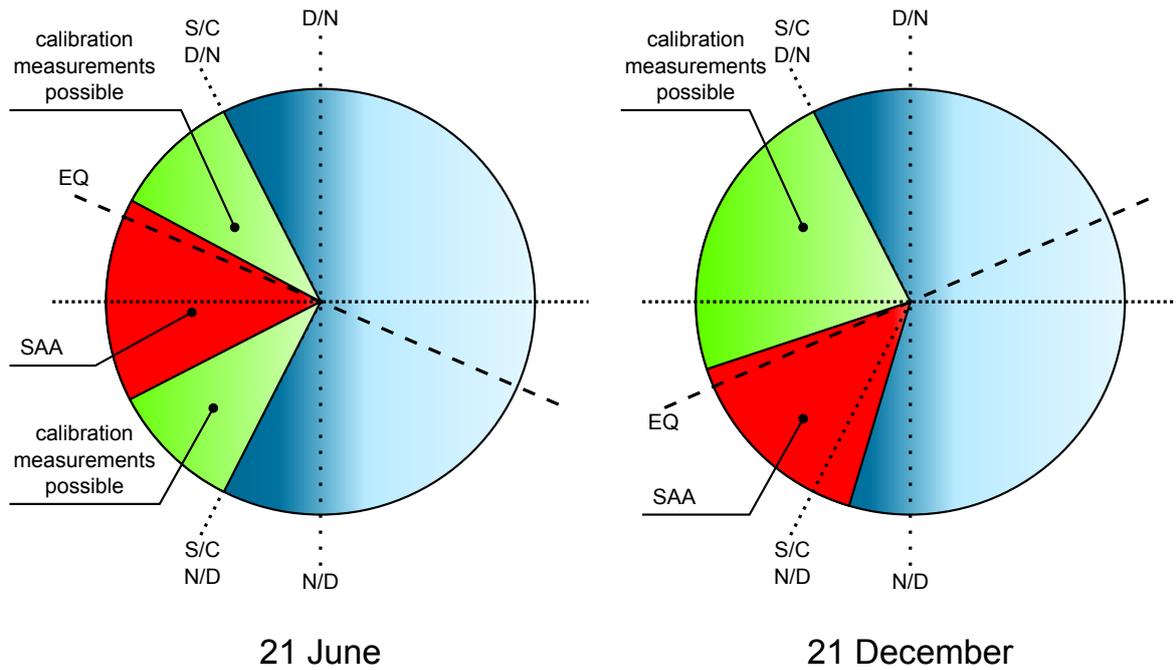


Figure 37: Seasonal variation of the SAA relative to the orbit. S/C = spacecraft, EQ = equator, SAA = South Atlantic Anomaly, D = day, N = night.

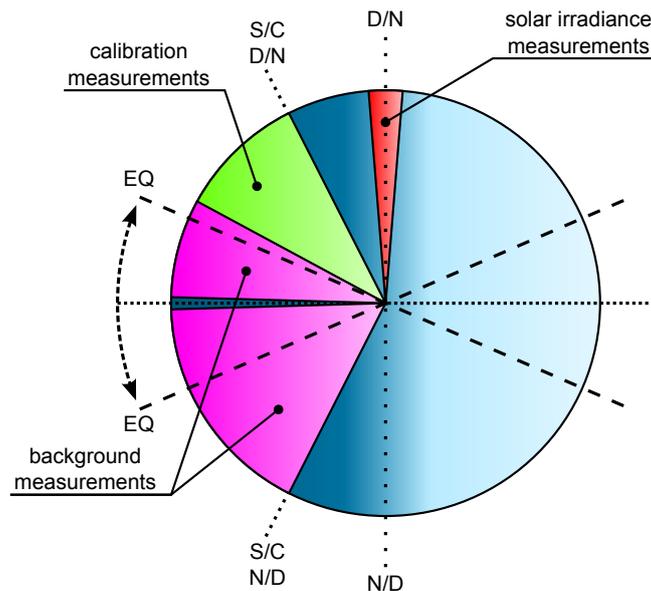


Figure 38: Position of irradiance, calibration and background measurements in the orbit. S/C = spacecraft, EQ = equator, SAA = South Atlantic Anomaly, D = day, N = night.

[1,65535]. This instrument configuration ID, or Icid, is primarily used by the instrument, where it identifies an entry in the instrument configuration tables. On ground the Icid is used to determine the intended purpose of a measurement and is used in the L01b data processing to determine the processing path.

For an Icid it is possible to have multiple versions, identified by the **instrument configuration version** or IcfVersion. The combination of Icid and IcfVersion uniquely identifies the set of configuration settings of the instrument. At a given time only one IcfVersion of an Icid can be active within the instrument. The IcfVersion allows to have multiple versions of a measurement with the same purpose, but with different settings. As a result of, for example, instrument degradation it may be required to change the settings for a measurement. In that case it is not necessary to create a new Icid, instead the same Icid can be using with a new IcfVersion.

The instrument settings are stored on-board in a hierarchical table structure as illustrated in Figure 40. At

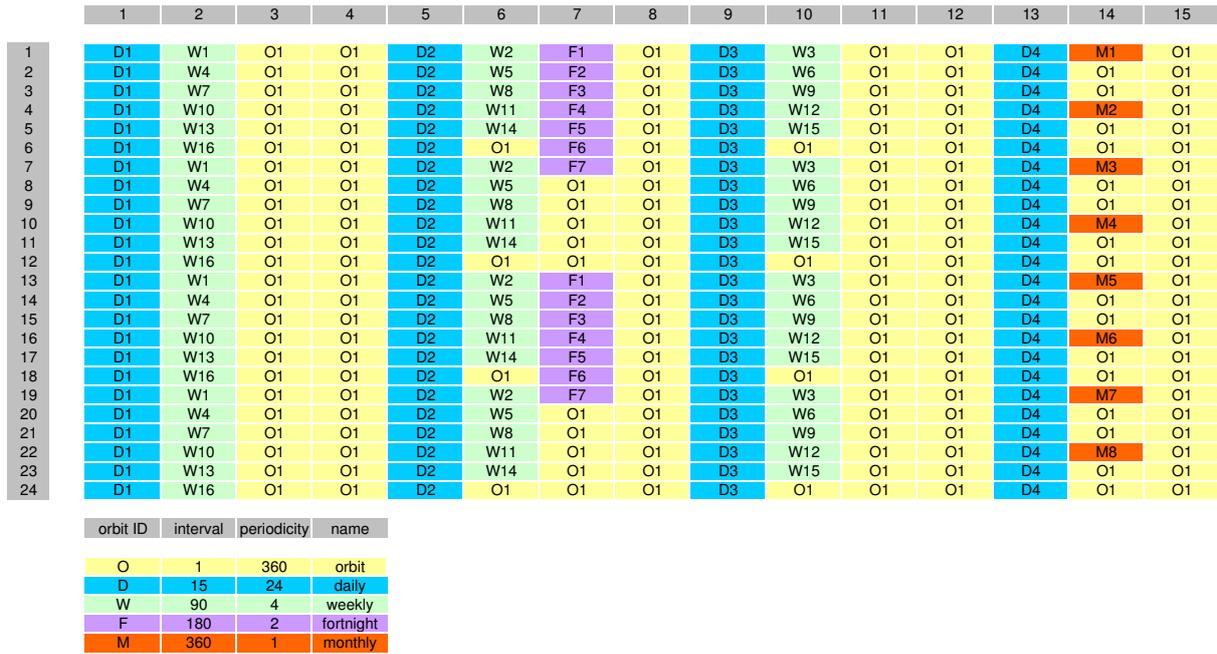


Figure 39: Nominal operations baseline overview. The schematic was retrieved from [RD9]. The horizontal direction shows the order of the 15 orbits in one S/C day. The vertical direction shows the different S/C days in one S/C month of 360 orbits. The different colors indicate the repetition cycle for the orbit types. The time in between measurements of one orbit-type is shown in the small table underneath.

the basis is the **measurement set collection**, which stores the configuration for each setting in a measurement set that is identified by the ICID and IcVersion. The measurement set in turn refers to four DEM table entries and four ISM table entries. The DEM tables contain the configuration for the four detector modules (DEMs). The ISM tables contain the configuration for the instrument specific modules (ISMs). These ISMs are responsible for commanding the detector modules and for collecting and processing all data from the detector modules.

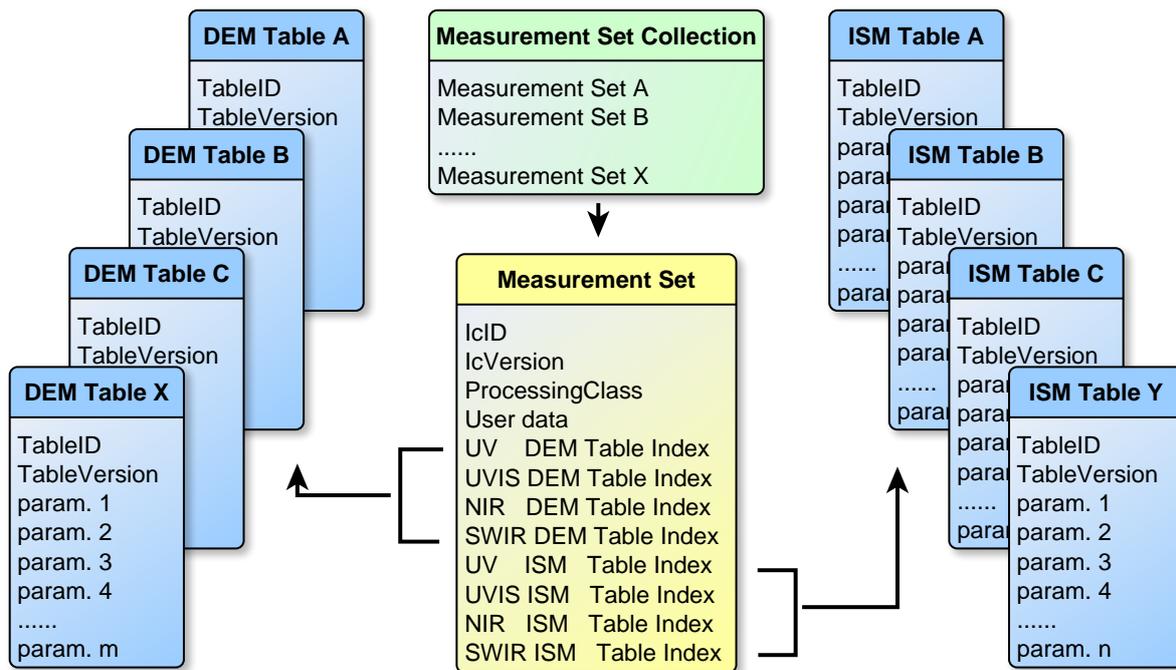


Figure 40: TROPOMI on-board instrument configuration structure.

13.2 Earth radiance measurements

The Earth radiance measurements form the bulk of the measurements. Apart from the optical properties of the instrument, there is some flexibility in the electronics that determines the Earth radiance ground pixel size. The co-addition period determines the ground pixel size in the along-track direction. Row binning (which is possible for UVN-DEMs only) determines the ground pixel size across-track. The parameter space is limited however, as choosing a smaller ground pixel size will increase the data rate and will decrease the signal-to-noise ratio for the individual ground pixels. The data rate is limited by both internal interfaces within the instrument as well as by the platform’s on-board storage and down-link capabilities.

For the Earth radiance measurements the co-addition period will be set to 1080ms. This effectively results in a ground pixel size of approximately 7km along-track. For the SWIR-DEM, which contains a CMOS detector, row binning is not supported. This means that, effectively, the binning factor is 1 for the SWIR bands (Band 7 and Band 8), resulting in a ground pixel size across-track between 7km at the center and 34km at the edges of the across-track field of view. The ground pixel size varies across-track since the spatial dispersion (degrees/pixel) is constant, resulting in a ground pixel size that becomes larger towards the edges of the across-track field of view due to the Earth’s curvature.

For the UVN-DEMs, binning factors are optimized to obtain a more constant ground pixel size across-track. For Bands 2, 3, 4, 5 and 6 a binning factor of 2 is used in the center and in a large region around it. At the edges of the across-track field the binning factor becomes 1. This results in a ground pixel size that varies between 3.5km and 15km where the latter value is reached for pixels just before the binning factor changes from 2 to 1. For Band 1 the binning factor is much higher in order to increase the signal-to-noise. In a region around the center, the binning factor is 16. On both sides an intermediate region with binning factor 8 exists, while the pixels near the edge have a binning factor of 4. This results in ground pixel sizes of 28km in the center and of 60km near the ‘8-4’ fault line.

Band	DEM	Binning factor	Across-track ground pixel size
1	UV	4...16	28 ... 60 km
2	UV	1...2	3.5 ... 15 km
3	UVIS	1...2	3.5 ... 15 km
4	UVIS	1...2	3.5 ... 15 km
5	NIR	1...2	3.5 ... 15 km
6	NIR	1...2	3.5 ... 15 km
7	SWIR	n/a	7 ... 34 km
8	SWIR	n/a	7 ... 34 km

Table 12: Binning factors and across-track ground pixel sizes for Earth radiance measurements.

The binning factors specified in Table 12 only apply to the part of the detectors that contain the spectrometer signals. For the UVN detectors, the spectrometer output only illuminates a part of the rows of the detector. The remaining rows are used for in-orbit calibration purposes. These calibration rows will be read out with higher binning factors in order to improve the signal-to-noise ratio and to reduce the instrument’s data rate.

Apart from the binning factor and the co-addition period, the remaining configuration parameters for the Earth radiance measurements, including exposure time and gains, will be optimized for the best signal-to-noise ratio, without causing saturation of the detector or electronics. This optimization will be based on scenes with the highest radiance levels, typically clouded scenes. Since the highest radiance level changes as a function of latitude, a total of five different settings for different latitude zones are created.

13.3 Solar irradiance measurements

The Sun is visible in TROPOMI’s solar irradiance port every orbit for a period of approximately 2 minutes around orbit phases 0.75, as illustrated in Figure 38. Every 15 orbits - approximately once every calendar day - TROPOMI will be commanded to perform a solar irradiance measurement. As the main purpose of the solar irradiance measurement is to calculate top-of-atmosphere reflectance, the solar irradiance measurement follows the same binning scheme as the Earth radiance measurements. The remaining parameters will be optimized for the best signal-to-noise ratio. The signal-to-noise ratio is improved even further by averaging the solar irradiance measurements within the L01b Processor.

13.4 Background measurements

The background signal for measurements will be calibrated in-orbit. For this to work, every measurement should have accompanying background measurements in the same orbit. These background measurements are performed using identical settings as the measurement they accompany. A different ICID for the background measurement ensures that on-ground it is being processed as a background measurement. The background measurements are performed on the eclipse side of the orbit as illustrated in Figure 38.

13.5 Calibration measurements

Calibration measurements will be performed on the night side of the orbit, outside the SAA, as illustrated in Figure 38. The binning scheme that is used for a calibration measurement depends on the objective of that measurement. Calibration measurements that have a strong relation with Earth radiance measurements will use the same binning scheme as Earth radiance measurements. These typically are measurements that focus on optical properties or that focus on instrument performance degradation. Most calibration measurements however will use a so-called unbinned scheme, that reads out all the pixels of the detector. For these measurements, the co-addition period may be slightly longer than for Earth radiance measurement, to avoid data rate bottlenecks within the instrument or the platform.

The other instrument configuration settings are typically optimized for the signal-to-noise ratio. For specific calibration purposes it is necessary to vary one or more parameters of the measurement. For example, to characterize the different gains of the instrument, a measurement series will be performed where the gain is varied, but all other settings are fixed.

14 Instrument calibration

Many of the algorithms presented in this document require calibration key data (CKD) as parameters. There can be several sources for these CKD parameters:

static Static parameters are parameters that have fixed values that are determined once, for example using design values, and never updated. Such parameters are typically not critical for the quality of the processed data and as such require no calibration.

on-ground calibration Parameters that are determined during the on-ground calibration campaign. Some CKD parameters can only be determined on-ground (e.g. absolute radiometric responsivity) and will from thereon be fixed for the entire mission. Other parameters can be calibrated in-flight as well and will be updated during the mission as necessary using in-flight calibration.

in-flight calibration Parameters that are determined using in-flight calibration measurements. The derivation of the CKD parameters from the in-flight calibration measurements is done in the payload data ground segment (PDGS) by special calibration processors, i.e. outside the L01b processor.

in-orbit calibration Parameters that are determined by the L01b processor using data from the orbit that is being processed. This is typically used for CKD parameters that vary or drift over the orbit or that are dependent on the scenery or the state of the instrument (e.g. instrument temperature). In-orbit calibration is fully handled internally by the L01b processor.

The degradation of the instrument is handled by updating the CKD parameters using in-flight calibration. The degradation correction will be described in [RD10] and related documents. This means that the L01b Processor does not model any degradation, nor does it need to know about any degradation. The degradation is modeled and characterized using external calibration processors that are executed in the PDGS. The PDGS will maintain an archive of all CKD parameters, each set of CKD parameters bound to a time interval. When processing the L0 data into L1b using the L01b data processor, the correct CKD parameters are staged that match the status and degradation of the instrument for the data being processed.

15 Data processing

Figure 41 shows the operational perspective of the L01b in the processing chain. The L01b ingests Level-0 data and calibration key data (CKD) and produces Level-1b data products. These Level-1b data products are used for Level-2 and calibration processing. The results of the calibration processing are updates to the calibration key data. The Level-1b output consist of the following data products:

Level-1b radiance The Level-1b radiance products contain the Earth radiance measurements, including annotation data such as geolocation. For each data granule, there is a data product for each of the eight bands. The radiance products are the main input for the Level-2 processors.

Level-1b irradiance The Level-1b irradiance products contain the averaged solar irradiance measurements, including annotation data. For each data granule, there is a data product for each of the two modules, UVN and SWIR. The Level-2 processors will use the irradiance products to calculate reflectance from the Earth radiance data. The irradiance data is used for calibration processing as well.

Level-1b calibration The Level-1b calibration products contain the calibration and background measurements, including annotation data, as well as any calibration data that are derived from radiance and irradiance measurements. For each data granule, there is a data product for each of the two modules, UVN and SWIR. The calibration products are the main input for the calibration processors who will use these products for generating updates to the calibration key data and for generating trending and monitoring products.

Level-1b engineering The Level-1b engineering products contain the instrument's engineering data converted to physical units. For each data granule, there is a single data product. The engineering products are input for the calibration processors who will use these products for generating updates to the calibration key data and for generating trending and monitoring products.

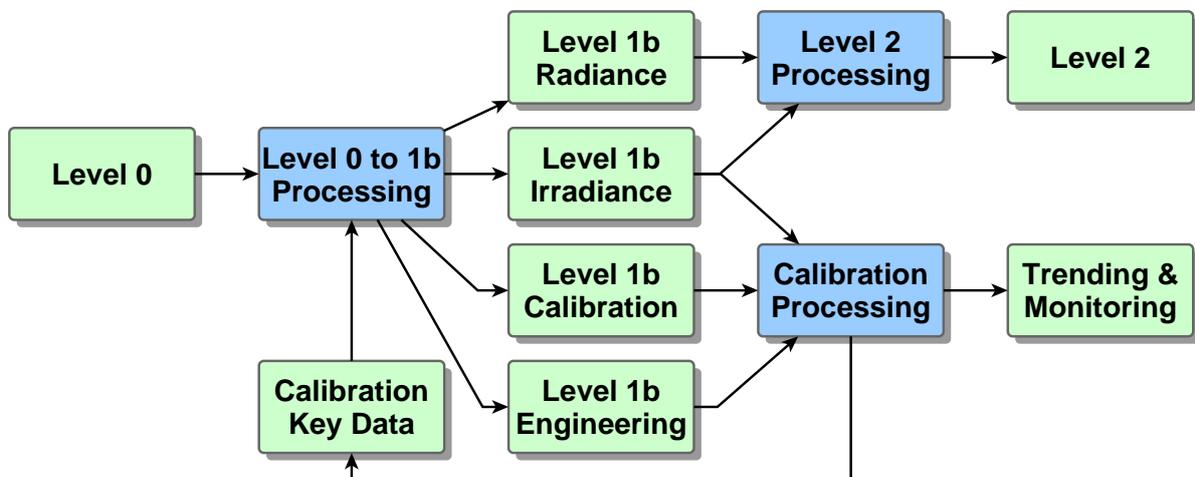


Figure 41: Operational perspective of the L01b, showing its data products and position in the processing chain. The blue blocks denote processors; the green blocks are data products.

The L01b Processor is operationally used in two different modes: **standard product processing** and **near-real-time (NRT) product processing**. The products from standard product processing have the highest quality but less stringent requirements for timeliness. This as opposed to the NRT products, which are required to be available within 2 hours 15 minutes after observation for L1b and 3 hours after observation for L2. To achieve this requirement, speed is favored over quality for the NRT products. The standard products can be distinguished from the NRT products by means of their product or file names.

During an orbit, all data generated by the instrument is stored on-board the spacecraft. When the spacecraft is visible for a polar ground station, once every orbit, the recorded data is downlinked. The data is then transferred from the ground stations to the **payload data ground segment (PDGS)** where it is processed. For NRT processing, it is essential that data is processed as quickly as possible. For this, the L01b Processor

processes the data as it comes in. For standard product processing this is different: The PDGS waits until all data for an orbit, from spacecraft midnight to spacecraft midnight, is present and only then starts the L01b processing. Waiting for a complete orbit and then processing it as a whole guarantees that all data required for in-orbit calibration is available. This results in the best possible products. For NRT products it is not guaranteed that all data for in-orbit calibration is available, resulting in products of lesser quality, but delivered within the timing constraint of 2h15 after observation for L1b products and 3 hours after observation for L2 products.

Part IV

Forward model

In this section, the TROPOMI instrument forward model is described. The forward model characterizes the signal as it propagates through the instrument, from the entrance aperture to the detector and then on to the read-out electronics. Based on this description, the correction steps performed by the L01b processor are identified and given in a mathematical formulation. This reverse model is presented in Part V. The forward model can be broken down into three sections: optics, detector and electronics. These are described below.

16 Optics

The optics of TROPOMI consists of a common telescope serving four spectrometers. Light from five different sources can enter the telescope, from where it propagates to the focal plane detectors.

First, a number of recurring symbols and equations used in this section are defined in the following table.

Parameter	Description	Units
λ	wavelength	nm
α	viewing angle across track	rad
t	time	s
$T_{\text{telescope}}$	transmission of the telescope	1
$A_{\text{telescope}}$	effective telescope aperture	m ²
A_{cu}	effective aperture of the calibration unit	m ²
$F_{\text{telescope,cross}}$	telescope focal length in the cross-track direction	m
$F_{\text{telescope,along}}$	telescope focal length in the along-track direction	m
P	polarization state	1
$T_{\text{scrambler}}$	transmission of the polarization scrambler	1
w_{slit}	slit size along track	m
$d\omega_{\text{slit}}$	solid angle at the slit	sr
S_{earth}	Earth spectral radiance	Wm ⁻² nm ⁻¹ sr ⁻¹
S_{sun}	solar spectral irradiance	Wm ⁻² nm ⁻¹
S_{wls}	spectral irradiance of the white light source	Wm ⁻² nm ⁻¹
S_{sls}	spectral irradiance of the spectral light source	Wm ⁻² nm ⁻¹
S_{cled}	spectral irradiance of the common LED	Wm ⁻² nm ⁻¹
S_{slit}	spectral flux at the slit	Wnm ⁻¹
θ_{sun}	incidence angle of the sun's light on the diffuser	rad
ϕ_{sun}	azimuth angle of the sun's light on the diffuser	rad
B_{diffuser}	bidirectional reflectance distribution function of the diffuser	sr ⁻¹
T_{optics}	transmission of the spectrometer optics	1
T_{grating}	transmission of the grating	1
T_{imager}	transmission of the imager optics	1
λ_b	band wavelength range	nm ⁻¹
G	line spread function or slit function: telescope, slit, and grating	nm ⁻¹
S_{grating}	spectral flux leaving the grating and reaching the detector	W

16.1 Telescope

The telescope can receive a signal from five radiative sources: the Sun, the Earth, the white light source, the spectral line source, and the common LED. The light path between the source and the telescope is different for each source, leading to different descriptions of the signal that arrives at the spectrograph slit (S_{slit}).

Earth radiance The telescope looks at the light radiated from and reflected by the Earth surface and atmosphere. The light enters through the Earth port (see Figure 14, top right panel), is depolarized by the polarization scrambler, propagates through the telescope, and reaches the slit. The signal at the slit is a function of wavelength, swath angle, and time:

$$S_{\text{slit}}(\lambda, \alpha, t) = S_{\text{earth}}(\lambda, \alpha, t, P) T_{\text{telescope}}(\lambda) T_{\text{scrambler}}(\lambda, P) A_{\text{telescope}} d\omega_{\text{slit}}, \quad (3)$$

where the across-track angle and the angle at the slit are related by

$$d\omega_{\text{slit}} = \arctan\left(\frac{w_{\text{slit}}}{F_{\text{telescope,along}}}\right) d\alpha. \quad (4)$$

The position on the slit in the across-track direction is related to the across-track angle through the corresponding telescope's focal length:

$$\alpha = \arctan\left(\frac{s_{\text{slit}}}{F_{\text{telescope,cross}}}\right), \quad (5)$$

where s_{slit} is the position along the slit. We note here that the polarization scrambler might have an effect on the exact shape of the point spread function when the scene is polarized, and that this might affect the geolocation algorithm. The effect is further discussed in Section 27. The contrast of a scene in along-track direction can have impact on the effective ISRF. The current understanding is that an altered ISRF can be modeled and fitted as part of Level 2 processing.

Solar irradiance The Sun's radiation, entering through the Sun port (see Figure 14, bottom right panel), reaches the telescope after having gone through one of two diffusers. The role of the diffuser is to reduce the intensity of the signal and make it comparable to the signal received from the Earth. At the slit the signal is:

$$S_{\text{slit}}(\lambda, \alpha, t) = S_{\text{sun}}(\lambda, t) \cos \theta_{\text{sun}} B_{\text{diffuser}}(\lambda, \alpha, \theta_{\text{sun}}, \phi_{\text{sun}}) T_{\text{telescope}}(\lambda) T_{\text{scrambler}}(\lambda) A_{\text{telescope}} d\omega_{\text{slit}}, \quad (6)$$

where ω_{slit} is as in Equation (4). Sun irradiance measurements are carried out by looking at the Sun while the spacecraft crosses the terminator from the day side to the night side. Because of this they are affected by a (non relativistic) Doppler shift. The apparent wavelength of the light is red-shifted according to

$$\lambda = \lambda_{\text{rest}} \left(1 - \frac{v}{c}\right), \quad (7)$$

where λ_{rest} is the rest wavelength, v is the component of the spacecraft velocity along the direction from the spacecraft to the Sun (taken to be positive when the spacecraft moves away from the Sun), and c is the speed of light in vacuum.

White light source The white light source is mounted inside the dedicated calibration unit and reaches the telescope when the selection mechanism is in the appropriate configuration (Figure 14, bottom left panel). The spectral flux at the slit for this source is:

$$S_{\text{slit}}(\lambda, \alpha, t) = S_{\text{wls}}(\lambda, t) T_{\text{telescope}}(\lambda) T_{\text{scrambler}}(\lambda) A_{\text{telescope}} d\omega_{\text{slit}}, \quad (8)$$

where ω_{slit} is again as in Equation (4).

Spectral Line Source] Similar to the white light source,

$$S_{\text{slit}}(\lambda, \alpha, t) = S_{\text{sls}}(\lambda, t) T_{\text{telescope}}(\lambda) T_{\text{scrambler}}(\lambda) A_{\text{telescope}} d\omega_{\text{slit}}, \quad (9)$$

where ω_{slit} is as in Equation (4).

Common LED The light from the common LED is diffused before reaching the telescope. So we have

$$S_{\text{slit}}(\lambda, \alpha, t) = S_{\text{cled}}(\lambda, t) B_{\text{diffuser}}(\lambda, \alpha) T_{\text{telescope}}(\lambda) T_{\text{scrambler}}(\lambda) A_{\text{telescope}} d\omega_{\text{slit}}, \quad (10)$$

where ω_{slit} is again as in Equation (4).

16.2 Spectrometer

The spectrometer projects an image of the slit on the detector while dispersing the signal in the spectral direction. The result can be described as a convolution of the transmitted slit signal and the slit function G . The slit function varies as a function of the swath angle α , due to the optics of the spectrometer (point spread function, aberrations, and defocussing) and small changes in the width of the slit. The changes in the slit cause a significant dependence of the slit function on the swath angle, and have to be accounted for in the processor (see Section 24.2). The form of the slit function determines the spectral resolution, as illustrated in Figure 42. Having introduced the slit function G , the signal received by the grating is:

$$S_{\text{grating}}(\lambda, \alpha, t) = \int S_{\text{slit}}(\lambda', \alpha, t) T_{\text{optics}}(\lambda') T_{\text{grating}}(\lambda) G(\lambda - \lambda', \lambda, \alpha) d\lambda'. \quad (11)$$

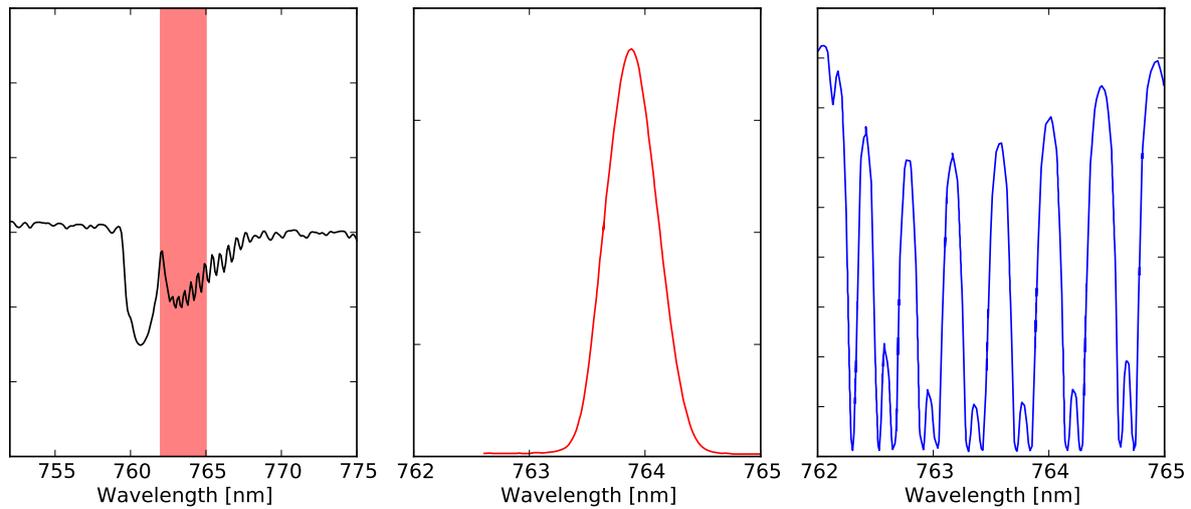


Figure 42: Illustration of the relative width of the slit function in comparison to the input radiance spectrum. The left panel shows incoming radiance, the wavelength region relevant for the other panels is shaded. The middle panel depicts the slit function and the right panel shows details of the input spectrum on the same scale as the slit function. The observed spectrum (not shown) is the convolution of the slit function with the input spectrum, and its resolution is dominated by the slit function.

16.3 Straylight

As described earlier in Section 10, the signal reaching each of the TROPOMI detectors contains a straylight (unintended) component caused by ghosting, scattering, and diffraction. For TROPOMI, straylight is a two-dimensional effect, occurring along both the spectral and the spatial directions.

The straylight contribution appears as an addition to the intended (useful) signal:

$$S_{\text{detector}}(\lambda, \alpha, t) = S_{\text{grating}}(\lambda, \alpha, t) T_{\text{imager}}(\lambda) + \int_{\lambda' \in \lambda_{\text{stray}}} \int_{\alpha' \in \alpha_{\text{stray}}} \int_{\beta' \in \beta_{\text{stray}}} S_{\text{stray}}(\lambda, \alpha, t, \lambda', \alpha', \beta') d\lambda' d\alpha' d\beta', \quad (12)$$

where the used symbols are described in the following table:

Parameter	Description	Units
λ, λ'	wavelength	nm
λ_{stray}	wavelength range that has an upper limit determined by the quantum efficiency of the detector of the spectrometer	nm
α, α'	across track angle	rad
α_{stray}	across track angle range which includes angles outside the field of view	rad
β, β'	along track angle	rad
β_{stray}	along track angle range which includes angles outside the field of view	rad
S_{grating}	useful signal leaving the grating and reaching the detector (straylight is not taken into account)	$\text{W nm}^{-1} \text{rad}^{-1}$
S_{stray}	straylight signal reaching the detector which is caused by the electromagnetic radiation at $(\lambda', \alpha', \beta')$	$\text{W nm}^{-2} \text{rad}^{-3}$
S_{detector}	total (useful + straylight) signal reaching the detector	$\text{W nm}^{-1} \text{rad}^{-1}$

17 Detector

TROPOMI employs two types of detector. For the three UVN chains, the detectors are CCDs (see Section 9.1.3), whereas the SWIR chain makes use of a CMOS device (see Section 9.2). Not only the physics of the detectors, but also their operation is different, and wherever necessary a distinction between the two will be made. In the following when we say *detector* we mean either the CCD or the CMOS; when one of the two is intended we say *CCD detector* or *CMOS detector*. The signal, including straylight, has now reached the detector. Here, charge is generated on a pixel location due to the incoming signal. Charge is also accumulated due to dark current. The charge is then transported towards one of the output nodes. During the transport the charge packet undergoes – depending on the detector type – several modifications, like smear, charge transfer inefficiency, and memory effect. We define in the following table a number of symbols recurring in the equations used in this section.

Parameter	Description	Units
λ	wavelength	nm
α	viewing angle across track	rad
t	time	s
R	pixel response function along the two axes of the detector	$\text{rad}^{-1} \text{mm}^{-1}$
Q	average quantum efficiency of the detector	1
U	pixel response non uniformity	1
S_{e^-}	electron flux in the pixel	$\text{e}^- \text{s}^{-1}$
T	detector temperature	K
$N_{\text{row,det}}$	number of rows in image part of the detector	1
$N_{\text{row,det,storage}}$	number of rows in storage part of the detector [†]	1
$N_{\text{det,binning}}$	binning factor applicable to a certain detector row [†]	1
t_{exp}	image exposure time	s
τ	row transfer time [†]	s
ε	charge transfer inefficiency [†]	1

[†] UVN detectors only.

17.1 Charge generation

We consider the generation of charge on a detector pixel $\mathbf{x}_{\text{det}} = (r_{\text{det}}, c_{\text{det}})$. There exists a mapping between the detector coordinates \mathbf{x}_{det} on the one hand, and the wavelength and viewing direction on the other hand:

$$(r_{\text{det}}, c_{\text{det}}) = (f(\lambda, \alpha), g(\lambda, \alpha)). \quad (13)$$

The right-hand side of this equation can in general not be simplified to $(f(\alpha), g(\lambda))$ due to the spectral and spatial *smiles* of the detector (these are caused by optical aberrations in the telescope and the optics).

We introduce the (normalized) pixel response function $R[\mathbf{x}_{\text{det}}]$ that implements this mapping. R will be elaborated on in section 26.4. The width of the pixel response function in row and column direction determines the sampling distances of a detector pixel. These distances, in turn, provide the limits in the integral in the equation below:

$$S_{e^-}[\mathbf{x}_{\text{det}}, t] = \iint_{\lambda, \alpha \in \mathbf{x}_{\text{det}}} S_{\text{detector}}(\lambda, \alpha, t) R[\mathbf{x}_{\text{det}}] Q(\lambda) U[\mathbf{x}_{\text{det}}] d\lambda d\alpha. \quad (14)$$

The product QU is the quantum efficiency of the detector, factored in two terms: Q is the average quantum efficiency, and U is the pixel response non-uniformity (PRNU). The latter is caused by differences in the pixel size and treatment of the detector surface leading to subtle pixel-to-pixel variations of the responsivity. At this stage, the detector has collected the incoming photons and converted them into packets of electrons, spatially confined in detector pixels.

A pixel also accumulates charge due to dark current (I_{dark}). The dark current contribution increases linearly with time and is in general a function of the temperature of the detector. Each pixel has a different dark current level.

The exact amount of dark current accumulated by a pixel depends therefore on the details of the pixel history, i.e. the time it takes for a pixel to be read out. This time is different for the CCD and the CMOS detectors. For a CCD detector, the total time the charge packet spends collecting dark current is determined by the transport time that follows from the charge life cycle (cf. Section 17.2). For the CMOS detector, the charge accumulated is read out immediately without any transfer, the charge accumulated is determined by the dark current rate and the exposure time only.

17.2 Charge transport

At the end of the exposure, the packets of electrons are transported to the read-out node, processed through the electronic chain, and digitized for later transmission to the ground. However, the physics, operations, and read-out schemes of the two types of detector are different (see Sections 9.1.3 and 9.2.3), which leads to two completely different life-cycles for the charge accumulated in a pixel. The following processes can add or remove charge to the amount of charge eventually read out as belonging to a given pixel: dark current, charge transfer inefficiency, image smear (i.e., charge due to light originating from other spatial pixels), or memory effect (i.e., charge left behind from the previous exposure).

Straylight (Section 16.3) is not dealt with explicitly here because by the time the photons have reached the detector it can no longer be distinguished from the genuine signal.

17.2.1 Charge life cycle in the CCD detectors

Consider the life cycle of the charge packet collected by a CCD pixel \mathbf{x}_{det} during an observation, as a function of time t :

- The initial charge is taken to be 0. We start the time counter here as $t = t_0 \equiv 0$.
- The packet enters the CCD column corresponding to \mathbf{x}_{det} from the frame side (top) of the CCD, at row $N_{\text{row, det}}$, and it reaches the detector row r_{det} after $N_{\text{row, det}} - 1 - r_{\text{det}}$ parallel transfers, each lasting τ seconds, taken to be the time that the charge packet resides in each row. When the charge packet reaches its proper row: $t = t_1$. During this time, the image section is already illuminated and dark current is being built up.
- The charge packet then resides t_{exp} in row r_{det} . This is the time interval proper when electrons are generated for the intended location. When the charge packet begins to be transported towards the output node $t = t_2$.
- The charge packet undergoes further r_{det} parallel transfers until it reaches the storage section of the CCD. Now $t = t_3$.
- Another $N_{\text{row, det, storage}}$ parallel transfers occur inside the storage section until the charge packet reaches the read-out register at $t = t_4$. The storage section is shielded from direct illumination; only dark current and charge transfer efficiency alter the charge content of a packet now.

- Before being serially transferred out of the read-out register, the charge packet resides another ($r_{\text{det}} \bmod N_{\text{det,binning}}$) parallel transfer times in the read-out register due to detector row binning: multiple CCD rows, are added in the read-out register. The number of adjacent rows that are combined can vary over the image and is determined by a binning table. Row binning is required to reduce the amount of data transferred to the ground. The related averaging process ('binning correction') that takes place in the L01b Processor reduces the variance of the signal. Now $t = t_5$.
- Finally, the charge packet is read out after $n_{\text{c}_{\text{det,ser}}}$ serial transfers, each lasting t_{ser} . The precise number of serial transfers is the distance, measured in columns, to the nearest output node. The two output nodes are located at the left and right endpoints of the ROR. Now $t = t_6$.

Note that dark current is being accumulated during all steps between t_0 and t_6 .

17.2.2 Charge life cycle in the CMOS detector

The charge life cycle for the CMOS detector is different. Each pixel has its own capacitive trans-impedance amplifier and sample and hold amplifier, and the CMOS detector therefore has no charge-transfer inefficiency or smear. However, for the CMOS detector, the actual amount of charge recorded by a pixel is affected by the illumination history (memory effect). The SWIR CMOS detector operates in integrate-while-read mode, whereby the charge accumulated during an exposure is read out while the next exposure takes place. This can lead to image artifacts.

17.2.3 Related effects

This section discusses three processes that alter the charge content of each package during transport.

Charge transfer inefficiency In CCD detectors, when a packet of electrons moves to the next pixel a small fraction of the charge in the packet is left behind, while simultaneously the packet picks up some charge left behind by preceding packets. The combined effect of subtractions and additions of charge are small and always result in a net charge loss. The evolution of the signal after the $(n + 1)$ th row or column transfer is described by

$$S_{n+1}[k] = (1 - \varepsilon)S_n[k] + \varepsilon S_n[k - 1] . \quad (15)$$

Here, k denotes the pixel number of the original location of the charge packet, while $k - 1$ is a pixel location one step upstream the transport direction. Basically, the repeated application of Equation (15) for all pixels, and after all transfers, provides the complete description of the CTE effect. This is elaborated on in the reverse model chapter (see 22.6).

Smear The CCD detectors have no shutter mechanisms. This means that the detector pixels are always collecting photons, including during the parallel transfers, thus between t_0 and t_1 and between t_2 and t_3 . This process leads to charge (photons) pick up from other spatial locations across track. The amount of extraneous charge collected by a pixel depends on the scene being looked at. While the phenomenon can be easily explained and understood, correcting for it is rather complex (see Section 22.10).

Memory effect Memory effects appear for the CMOS detector when the signal level changes between successive exposures. The signal is higher or lower than expected if the previous exposure had a higher or lower signal level.

18 Electronics

We now follow the signal of a single pixel as it travels through the electronic chain, from the detector to the digitization unit. We can subdivide the chain in three stages: conversion from charge to voltage, amplification and conditioning, and finally digitization. In Figure 43, the UVN chain is graphically depicted. There is one read-out circuit per UVN band.

For the SWIR chain, as shown in Figure 44, parts of the read-out chain are per pixel, and parts per detector quarter, corresponding to half a detector band.

Note that the signal is now defined in terms of image pixels \mathbf{x}_{img} instead of detector pixels \mathbf{x}_{det} since, for CCDs,

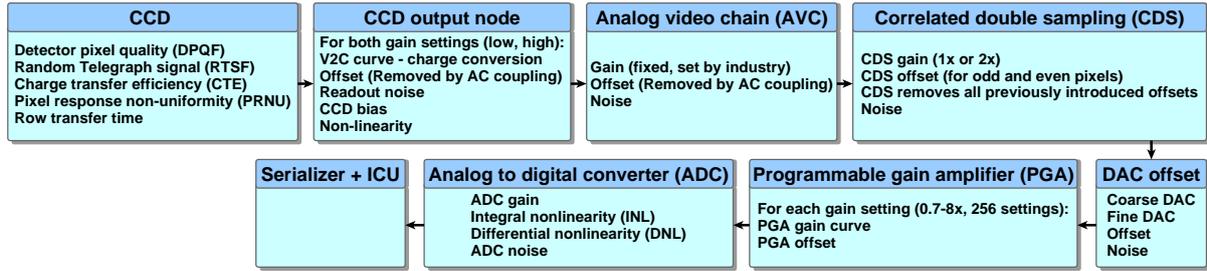


Figure 43: The different components of the read-out chain of the UVN detectors with their respective contributions to the signal. Each UVN detector band has its own output node and read-out chain.

detector rows may have been binned in the read-out register before the serial column transfers to the output node of the detector.

We define in the following table a number of symbols recurring in the equations used in this section.

Parameter	Description	Units
$S[\mathbf{x}_{img}]$	image pixel signal before conversion	e^-
$S'[\mathbf{x}_{img}]$	image pixel signal after conversion	V
$N_{nl}(S[\mathbf{x}_{img}])$	non-linearity function	1
G_{c2v}	detector gain = output amplifier responsivity	$V(e^-)^{-1}$
O_{c2v}	detector offset	V
G_{avc}	Analog video gain	VV^{-1}
G_{cds}	CDS gain [†]	VV^{-1}
O_{cds}	CDS offset [†]	V
G_{pga}	programmable gain [†]	VV^{-1}
O_{pga}	offset due to PGA gain [†]	V
O_{dac}	programmable offset [†]	V
G_{adc}	ADC gain	DNV^{-1}
n_{coadd}	Number of co-additions	1

[†]UVN detectors only.

18.1 Charge-to-voltage conversion

For the **UVN** chains, the charge-to-voltage conversion consists of the following steps:

Non-linearity Non-linearities occur at different steps in the electronic chains. For UVN, the main source of non-linearity can be located at the CCD output node. We model this by applying to the signal a non-linearity function. Instead of the simple multiplication relation that can be expressed as a straight line, the combined application of both non-linearity and the conversion can also be regarded graphically as a voltage-to charge *curve*:

$$S'[\mathbf{x}_{img}] = N_{nl}(S[\mathbf{x}_{img}]) . \tag{16}$$

The non-linearity function may depend on the voltage-to-charge gain setting.

Conversion to voltage The actual conversion takes place in the CCD output node. There are two gain settings. Each gain setting also introduces an offset, the CCD bias:

$$S'[\mathbf{x}_{img}] = S[\mathbf{x}_{img}]G_{c2v} + O_{c2v} . \tag{17}$$

Video amplification Additionally, there is also a video amplification stage. The amplification provided by this stage is fixed at FEE construction time and cannot be changed. The AVC will also introduce a nonlinearity, but

this is expected to be negligible compared to the CCD output node nonlinearity. An offset belonging to this step, if present at all, is expected to remain constant and will be invisibly incorporated in other offsets:

$$S'[\mathbf{x}_{\text{img}}] = S[\mathbf{x}_{\text{img}}]G_{\text{avc}} . \quad (18)$$

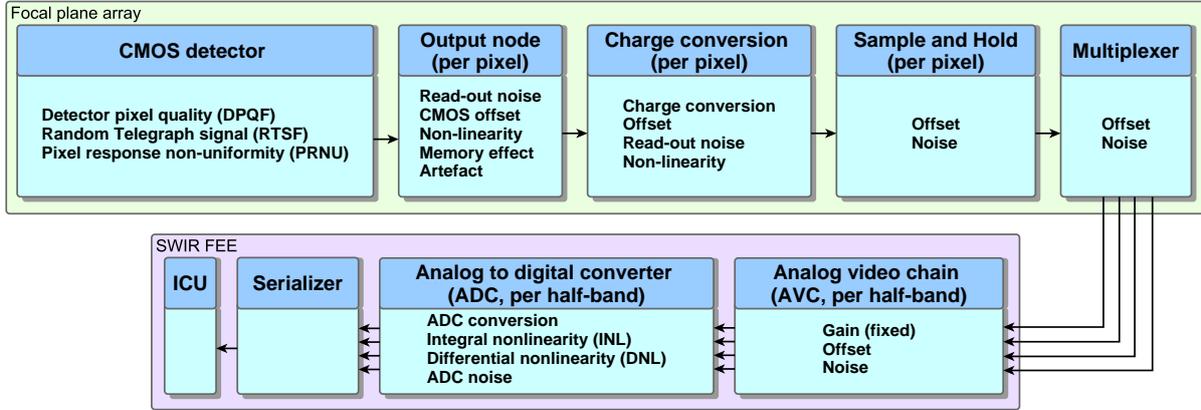


Figure 44: The different components of the read-out chain of the SWIR detector with their respective contributions to the signal. The read-out integrated circuit (ROIC) is directly connected to the detector pixels via indium bumps.

For the **SWIR** chain, as shown in Figure 44, the charge-to-voltage conversion consists of the following steps:

Non-linearity Non-linearities occur at several places in the read-out chain. Mathematically these are expressed as in the case of UVN, but the non-linearity can differ per pixel, as each pixel has its own output stage.

$$S'[\mathbf{x}_{\text{img}}] = N_{\text{nl}}(S[\mathbf{x}_{\text{img}}]) . \quad (19)$$

Conversion to voltage The charge to voltage conversion is performed per pixel in the capacitive trans impedance amplifier, leading to a pixel dependent conversion factor and offset. As the pixels are very similar, the conversion factor is taken identical for all pixels.

$$S'[\mathbf{x}_{\text{img}}] = S[\mathbf{x}_{\text{img}}]G_{\text{c2v}} + O_{\text{c2v}} . \quad (20)$$

Video amplification As in the UVN, there is a video amplification stage with the same characteristics:

$$S'[\mathbf{x}_{\text{img}}] = S[\mathbf{x}_{\text{img}}]G_{\text{avc}} . \quad (21)$$

18.2 Amplification and conditioning

Once the electron signal is converted to a voltage, it is amplified and conditioned before being presented to the analog-to-digital converter for digitization.

For the **UVN** modules, the following steps apply:

Correlated double sampler The signal is processed through a correlated double sampler in order to eliminate fixed pattern noise. The process doubles the variance of the signal, but this variance increase is much less than it would be if this step were not applied. This process also introduces an offset dependent on the CDS gain chosen:

$$S'[\mathbf{x}_{\text{img}}] = S[\mathbf{x}_{\text{img}}]G_{\text{cds}} + O_{\text{cds}} . \quad (22)$$

Programmable offset In the next step, the signal arrives at an offset that actually can be controlled. This DAC offset is controlled by a coarse and a fine dial, allowing for an almost continuous range of offset setting:

$$S'[\mathbf{x}_{\text{img}}] = S[\mathbf{x}_{\text{img}}] + O_{\text{dac}} . \quad (23)$$

Programmable gain The programmable gain can be set in 256 steps. However, this gain will also introduce an offset depending on the PGA gain chosen:

$$S'[\mathbf{x}_{\text{img}}] = S[\mathbf{x}_{\text{img}}]G_{\text{pga}} + O_{\text{pga}} . \quad (24)$$

For the **SWIR** the conditioning is performed with fixed settings:

The amplifier in the video chain adapts the output signals of the detector to fit within the ADC input range. There are four video signals (for each detector half-band) with each their own gain and offset.

18.3 Digitization

After amplification and conditioning the signal is digitized by an analog-to-digital converter. This can be subdivided in two steps.

ADC The unit of the signal now changes to digital numbers. Note that, for the CCDs, the combination of the programmable gain and offset should have projected the signal to a suitable, non-negative range:

$$S'[\mathbf{x}_{\text{img}}] = S[\mathbf{x}_{\text{img}}]G_{\text{adc}} . \quad (25)$$

The noise stemming from digitization will be part of the read-out noise; the latter is a CKD.

For SWIR, it is possible that G_{adc} includes a non-linearity function.

Co-addition Finally, a number of subsequent individual detector images will be co-added in the co-addition register of the ICU. This action decreases the amount of data to be sent to the ground:

$$S'[\mathbf{x}_{\text{img}}] = \sum_{n_{\text{coadd}}} S[\mathbf{x}_{\text{img}}] . \quad (26)$$

During this step any temporal signature of the signal on time scales shorter than the co-addition period is lost, but for data from the small-pixel columns (one per detector). These are transmitted to the ground without being co-added, and can be used for monitoring purposes or to adjust calibration parameters.

Part V

Reverse model

In this section we deal with the L01b Processor properties. The starting point of the processor is the Level-0 data as received from the ground system. The main component of this input is the measurement data, or signal, S , expressed in digital numbers (DN).

Through a number of correction and calibration steps – referred to as ‘algorithms’ in this document – this digitized signal is transformed to give an estimate of the input stimulus that caused the measured signal, i.e., the Earth, the Sun, or one of the on-board light sources. Together with the signal, its variance σ^2 is also calculated and propagated through the L01b Processor. Details of the variance propagation algorithms, and especially the theoretical justification, are given in [AD3]. The output is Level-1b data that includes geolocated and calibrated radiances, calibrated irradiances, and calibration measurement results.

After a description of the processing flow (Section 19) and some general remarks (Section 20) the remainder of this part describes the algorithms in detail, by giving for each algorithm the two main equations that describe the transformations of the signal and its variance per image pixel. Where needed, these are augmented by auxiliary equations and a table summarizing all the symbols used. The sections in this part are organized according to the division in generic and module specific algorithms.

19 Processing flow

In the L01b Processor, the various calibration and correction algorithms are traversed in a well-defined order (Figure 45). Some algorithms are shared by all detectors (Figure 46), while others apply only to the UVN modules (Figure 47) or the SWIR module (Figure 48). None of the algorithms makes a functional difference between bands; hence none of the equations use a subscript b . However, the calibration key data may differ between bands.



Figure 45: An overview of the processing order in the Level 1b processor. Instrument features that affect all detectors are corrected for in the generic corrections (see Figure 46). In the module specific corrections the features that only affect the UVN or SWIR detectors are addressed (see Figures 47 and 48).

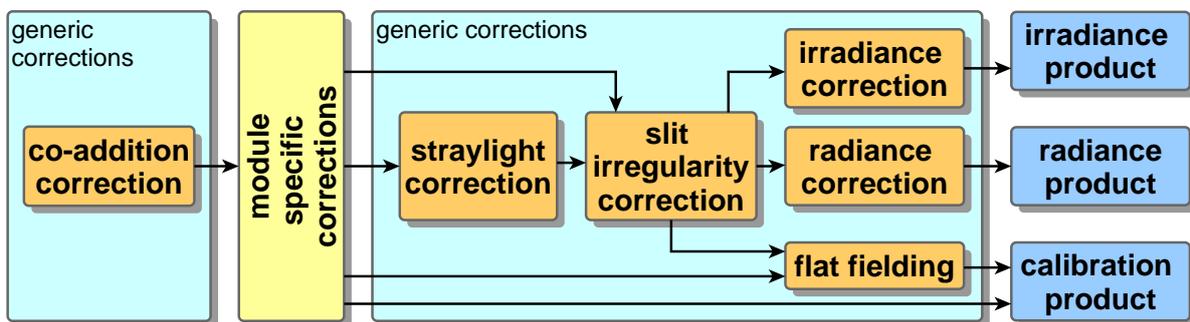


Figure 46: Instrument features that affect all detectors are corrected for in the generic corrections in the Level 1b processor. The algorithms used in the generic corrections are identical for all detectors, however the calibration key data parameters may differ per detector band. In this schematic the flagging algorithms are omitted.

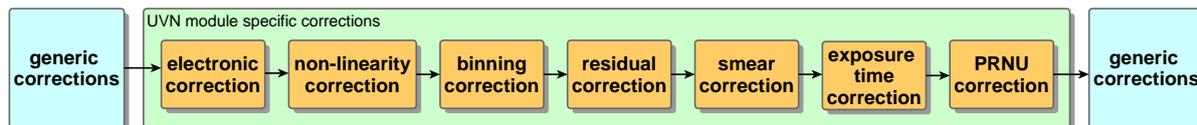


Figure 47: The UVN specific corrections in the Level 1b processor. The flagging algorithms are omitted in this schematic.

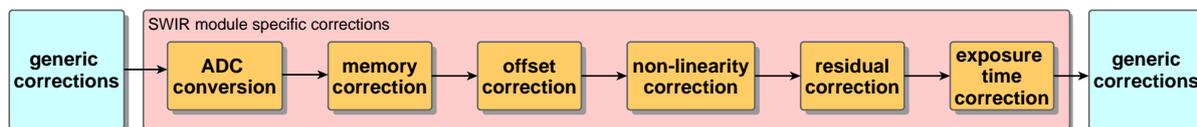


Figure 48: The SWIR specific corrections in the Level 1b processor. The flagging algorithms are omitted in this schematic.

19.1 Rationale behind the order of the algorithms

In determining the processing order of the algorithms, the main rule is that the reverse model is, literally, the reverse of the forward model. All physical processes described in the forward model chapter are expressed mathematically and the algorithm step for the reverse model is the inverse operation. That means, for example, that the conversion from volts to digital numbers near the end of the forward model (the ADC converter) becomes, near the start of the reverse model, a conversion from digital numbers to volts. There are several exceptions to this main rule, for a number of reasons. Because the amount of information in the forward model decreases, some steps do not have a proper inverse. Further, some processes are not concentrated in time or space (e.g. straylight) while for the correction algorithm a well-defined position in the processing flow has to be chosen. Below, we describe all processes, and the concerning decisions, that are not covered by the main rule (i.e. simple inversions of the forward model).

Co-addition division Information of the original measurements is lost in the adding operation in the forward model. An average original image is assumed here.

Gains and offsets The electronic chain is characterized by a combination of partial gains and offsets. After combination, a total electronic gain and electronic offset can be determined. These depend on the instrument settings, denoted by the gain-and-offset code \mathbf{g}^* . That is, the combined operation in the reverse model gives $S' = G(\mathbf{g}^*) \cdot S - O(\mathbf{g}^*)$. The notation implies that the order of correction is: first gain, then offset. This is, however, completely equivalent to $S' = G(\mathbf{g}^*)(S - O'(\mathbf{g}^*))$ where $O = GO'$. Because both gain and offset are functions of \mathbf{g}^* , the choice does not matter. In the calibration, the offset O' is found by setting $S = 0$. Therefore, the chosen order in the reverse model is: first offset, then gain.

Memory effect and artifacts These SWIR algorithms correct for features in electronics and the reading cycle and appear therefore early in the chain. The precise locations of these two additive corrections is not important as long as they are consistent with the related calibration measurements.

Voltage-to-charge and non-linearity At the output node of the CCD, the signal, in the forward sense, is converted from electrons to volts. This conversion is not entirely linear. The amount of non-linearity can be described by a dimensionless transfer function $f(S)$ where $f(S) \equiv 0$ implies pure linear behavior. We have chosen to separate the unit conversion from the non-linear behavior; hence the non-linearity function $f(S)$ is from electrons to electrons.

Binning In a similar approach as for co-addition correction, an average signal over the concerned rows is assumed here. The position of this algorithm is after the non-linearity correction, since the latter operates on the total signal. The algorithm should not be moved to a later position because row-to-row signal continuity is preferable (if only for visualization purposes).

Transient pixel flagging This algorithm is different from the two other quality-related algorithms: detector pixel quality and RTS. Those algorithms use CKD maps. The timescale for transient behavior is such that it can only be detected between measurements. The position of the algorithm in the L01b processing flow should be such that the signal be corrected as much as possible, but before the smear correction (the computation of smear cannot take transient pixels into account; it has to treat them as skipped pixels).

An idea is to place the transient flagging algorithm after the residual correction to ensure that the transient behavior only needs to be investigated on the combined (i.e. illuminated minus residual) image. However, the quality of the dark current and residual CKD is such that transients will not be present there. Therefore it is more logical to position the transient flagging algorithm immediately before the dark current correction algorithm.

Dark flux/dark current and residual correction The dark current CKD is defined per unbinned pixel. A non-illuminated image is defined as the sum of dark current (and, in the case of SWIR, thermal background) and a residual term. Per construction, dark current/dark flux is subtracted first from both the actual illuminated measurement and its associated background measurement. By definition, the corrected background measurement now only contains a residual. This residual is then subtracted from the corrected illuminated measurement. The processing flow for the background measurement ends here since nothing of that image is left.

Smear The correction of smear can take place when all offsets have been removed. Because the smear is, in mathematical sense, a linear operator, the position of this algorithm does not have to move towards the beginning; in particular, smear correction for dark current (and, possibly, residual) on both illuminated and dark images is not necessary since these smear terms cancel in the previous residual algorithm. On the other hand, this is the latest position where the exposure time is needed in an algorithm.

PRNU and slit irregularity The associated CKDs are derived in the same calibration algorithm. Due to their associated locations in the instrument, they are dealt with in this order. Note that the PRNU for SWIR is redundant since the SWIR nonlinearity is pixel-dependent.

Straylight The processes that lead to straylight cannot be pinpointed to a particular location in the instrument. However, we can argue that (internal) straylight occurs between the entrance slit and the detector. Therefore its correction is between PRNU correction and slit irregularity correction. Moreover, the straylight correction assumes linear behavior of the signal, necessitating its position after PRNU correction.

Spectral annotation An initial spectral annotation (also called wavelength assignment), derived from ray-tracing simulations of the optical model, is performed at the start of the processing chain. On the other hand, improved spectral annotation (namely, spectral fit after Doppler correction for irradiance) can best be performed on the useful signal, after slit irregularity. Note that the straylight correction algorithm is based on a pixel-to-pixel transfer matrix and does not need spectral information.

20 General remarks

20.1 Signal propagation and flagging

The signal S is propagated in the L01b Processor from one algorithm to the next: the output signal S_o of one algorithm is the input signal S_i for the next. However, signal values are used in an algorithm depending on an assessment of their quality. This quality assessment is performed in a number of so-called flagging algorithms that assign quality flags and quality numbers to image pixels, ground pixels, or measurements. See Section 29 for more information on quality assessment.

The philosophy in the algorithms of the L01b is that it calculates correction parameters using only image pixels that may be considered reliable. That is, image pixels that are flagged 'defective' or 'missing', or for which a processing error has occurred in a previous correction algorithm, may not occur on the right-hand side of an equation describing the correction of another pixel.

On the other hand, the calculated correction parameters are applied to *all* image pixels, even those with errors. Even though the signal values for such image pixels are not useful for scientific purposes, they may

still be of use for calibration purposes. Thus, flagged pixels may occur on the left-hand side of an equation describing the current correction algorithm. The exception is that image pixels for which data is missing, are not corrected.

Like the signal and the noise, the quality flags are also propagated through the L01b Processor; i.e., they are updated if in a particular algorithm certain conditions are met. At the end of processing, quality assessment information is added as annotation data to the Level-1b data products so that users may use it to assess the quality of the Level-1B data and filter them before use.

20.2 Measurement noise propagation

We described in Section 5.1.2 the two types of measurement noise. We now elaborate on their role in the reverse model.

Read-out noise Read-out noise can be administrated in the reverse model once the signal has passed, in the reverse sense, the electronic circuit and is defined in electrons. This is immediately after the non-linearity correction in both UVN and SWIR. The read-out noise $\epsilon_{\text{readout}}^2$ can be acquired from a CKD or by using data from the current measurement. In both cases, we have to take the number of co-additions of the current measurement into account, see below. The noise depends on the band and the gain setting (and, for the SWIR detector, the pixel location). However, it does not depend on the magnitude of the signal. Introducing the read-out noise halfway in the processing flow requires the unit conversion algorithms later in the processing flow to also convert this noise. The binning division algorithm does not play a role here since this noise occurs at the read-out node. Other elementary correction algorithms do not influence the read-out noise: only the signal changes, while the read-out noise has already been defined.

Shot noise The shot noise can be computed once, in the forward model sense, the number of photons from the Sun have been converted to electrons and the signal has been corrected for effects that are independent of the generated amount of electrons. We can therefore choose to establish the shot noise somewhere between the end of the voltage-to-charge algorithm and the start of the exposure time division. It can be argued that we want to start with the signal that has undergone the smallest number of corrections, since that signal has actually been measured. Hence the choice to inject the noise directly after the voltage-to-charge algorithm. In this way, we count the number of electrons in a large, binned pixel. Moreover, this point coincides with the location of read-out noise injection.

Note that another location choice (e.g. after the smear correction algorithm) will alter the signal-to-noise ratio slightly, but has otherwise no large impact since binning effects cancel.

20.3 Noise propagation in forward and reverse directions; rules and characteristics

Our goal is to define the noise at each stage in the reverse model. In particular, we need values for the shot noise and read-out noise near the start of the reverse model. In order to do that, we must follow the path, in the forward model, from the ‘creation’ of the noise towards the end (when the signal is actually read). In these forward steps, we consider the physical changes that occur, such as conversions and the co-addition of several signals into one combined signal. The measurement noise in these steps is expressed algebraically (as a function of signal, instrument settings and CKDs), since we do not know the actual signal and CKD yet. At the end of the forward model, we can read the signal in digital numbers; only then can we define the start value for the measurement noise. Then, following the reverse model, we can propagate the measurement noise, along with the signal in a purely mathematical way, both algebraically and explicitly.

We use the following assumptions:

Shot noise is defined as the noise of a measurement, measured in electrons, registered by a binned pixel \mathbf{x}_{img} . The value of the shot noise (expressed as variance, with unit electrons squared) is equal to the number of electrons of the signal (in electrons) itself. It does not matter if we consider the shot noise of a large binned pixel or the n_{bin} shot noise values of the original detector pixels (each with its own signal S_i). In the first case, the shot noise equals $s_{\text{shot}}^2 \{\sum_{\text{bins}} S_i\} = \sum_{\text{bins}} S_i$. In the second case, the total shot noise is $\sum_{\text{bins}} s_{\text{shot}}^2 \{S_i\} = \sum_{\text{bins}} S_i$. Note that we use the bracket notation $\{\dots\}$ to link the noise to the signal at a certain stage (see also the symbol table below).

Read-out noise is the noise, measured in volts, at the read-out node. It depends on the electronic settings: gain and offsets. It is always measured for a binned pixel (signals are per definition binned before they are read out). Alternatively, the read-out noise can also be expressed in electrons (this is just a standard conversion) to align it with the shot noise.

Propagation of noise is purely mathematical for multiplicative algorithms in the reverse model, in particular the algorithms where the unit of the signal changes. There are no rules to cope with additive algorithm steps. In this way, the signal-to-noise ratio along the entire algorithm chain will approximately be the same, except for signals where offset contributions are relatively large.

Parameter	Description	Units
$S_{i,\text{source}}$	Signal generated at binned pixel, un-coadded measurement	e^-
$S_{i,\text{DN}}$	Signal propagated towards read-out node, un-coadded measurement	DN
$S_{\text{meas},\text{DN}}$	Co-added signal, at start of reverse model, as measured	DN
S'_{DN}	Signal after co-addition correction	DN
S'_{source}	Signal after voltage-to-charge correction	e^-
$S'_{\text{corr-bin}}$	Signal after binning correction	e^-
$S'_{\text{corr-dc}}$	Signal after dark current correction, before residual correction	e^-
$S'_{\text{res,corr-dc}}$	Residual signal before residual correction	e^-
$S'_{\text{corr-res}}$	Signal after residual correction	e^-
$s_{\text{meas}}^2 \{S_{i,\text{source}}\}$	Measurement noise, when created, of a single measurement	e^{-2}
ϵ_{ckd}^2	read-out noise as CKD parameter	e^{-2}
$s_{\text{meas}}^2 \{S_{i,\text{DN}}\}$	Measurement noise, propagated towards read-out node, of a single measurement	DN ²
$s_{\text{meas}}^2 \{S_{\text{meas},\text{DN}}\}$	Measurement noise of co-added signal, start of reverse model	DN ²
$s_{\text{meas}}^2 \{S'_{\text{DN}}\}$	Measurement noise of after co-addition correction	DN ²
$s_{\text{meas}}^2 \{S'_{\text{source}}\}$	Measurement noise after voltage-to-charge correction	e^{-2}
$s_{\text{meas}}^2 \{S'_{\text{corr-bin}}\}$	Measurement noise after binning correction	e^{-2}
$s_{\text{meas}}^2 \{S'_{\text{res,corr-dc}}\}$	Measurement noise of an aggregated residual signal	e^{-2}
$s_{\text{meas}}^2 \{S'_{\text{corr-res}}\}$	Measurement noise after residual correction	e^{-2}

We consider a binned pixel of a measurement S_i , $1 \leq i \leq N_{\text{coadd}}$ that is part of a co-addition. We start, in forward sense, at the read-out register with the signals $S_{i,\text{source}}[\mathbf{x}_{\text{img}}]$. These signals are measured in electrons (e^-). The measurement noise, defined as the sum of read-out noise and shot noise, is:

$$s_{\text{meas}}^2 \{S_{i,\text{source}}\}[\mathbf{x}_{\text{img}}] = S_{i,\text{source}}[\mathbf{x}_{\text{img}}] + \epsilon_{\text{ckd}}^2[\mathbf{x}_{\text{img}}] \quad \text{in } e^{-2}. \quad (27)$$

Here we use the fact that the shot noise variance is equal to the signal itself. Note that for UVN, the read-out noise is independent of the pixel location. That having said, we will omit the index $[\mathbf{x}_{\text{img}}]$ in the remainder of the section. Further, it has no frame index i attached since its estimation stems from previous data: it is a CKD parameter.

Proceeding in forward direction, the signal undergoes some conversions to arrive in digital units at the start of the co-addition register. These conversions are, in this order: conversion from charge to voltage; the multiplication by relative and absolute gain; and the conversion from voltage to digital numbers. The conversions are lumped together in a factor k ; the measurement noise, therefore, is multiplied by a factor k^2 . More specifically:

$$S_{i,\text{DN}} = kS_{i,\text{source}}, \quad (28)$$

$$s_{\text{meas}}^2 \{S_{i,\text{DN}}\} = k^2(S_{i,\text{source}} + \epsilon_{\text{ckd}}^2). \quad (29)$$

Then, all N_{coadd} signals are added together to one signal that is actually measured: $S_{\text{meas},\text{DN}}$. For the measure-

ment noise, we use the summation rule for uncorrelated variables.

$$S_{\text{meas,DN}} = \sum_{i=1}^{N_{\text{coadd}}} S_{i,\text{DN}} = k \sum_{i=1}^{N_{\text{coadd}}} S_{i,\text{source}} , \quad (30)$$

$$\begin{aligned} s_{\text{meas}}^2 \{S_{\text{meas,DN}}\} &= \sum_{i=1}^{N_{\text{coadd}}} s_{\text{meas}}^2 \{S_{i,\text{DN}}\} = k^2 \sum_{i=1}^{N_{\text{coadd}}} (S_{i,\text{source}} + \epsilon_{\text{ckd}}^2) \\ &= k S_{\text{meas,DN}} + k^2 N_{\text{coadd}} \epsilon_{\text{ckd}}^2 . \end{aligned} \quad (31)$$

Note that ϵ_{ckd}^2 is still defined in e^{-2} . Equation (31) immediately provides the starting values for the shotnoise and the read-out noise; we only need the measured signal in DN, the read-out noise CKD in electrons, the total conversion factor from electrons to digital numbers and the co-addition number. Note that the total conversion factor will depend on the electronics settings, more specific the combination of gain settings (denoted by the gain code \mathbf{g}): $k = k(\mathbf{g})$.

From now on, we follow the reverse model back to where we started. We have a single signal and its propagation is purely mathematical. Likewise, the related noise is propagated in the multiplicative algorithms.

First, the co-addition division gives a factor $1/N_{\text{coadd}}^2$ in the measurement noise.

$$S'_{\text{DN}} = \frac{1}{N_{\text{coadd}}} S_{\text{meas,DN}} , \quad (32)$$

$$\begin{aligned} s_{\text{meas}}^2 \{S'_{\text{DN}}\} &= \frac{1}{N_{\text{coadd}}^2} (k S_{\text{meas,DN}} + k^2 N_{\text{coadd}} \epsilon_{\text{ckd}}^2) \\ &= \frac{1}{N_{\text{coadd}}} (k S'_{\text{DN}} + k^2 \epsilon_{\text{ckd}}^2) . \end{aligned} \quad (33)$$

Then, the inverse conversion to electrons cancels the factor k^2 . Therefore, the signal and the measurement noise at the injection point after the voltage-to-charge conversion algorithm are defined as

$$S'_{\text{source}} = \frac{1}{k} S'_{\text{DN}} , \quad (34)$$

$$s_{\text{meas}}^2 \{S'_{\text{source}}\} = \frac{1}{N_{\text{coadd}}} (S'_{\text{source}} + \epsilon_{\text{ckd}}^2) . \quad (35)$$

Here we have another good point to establish the measurement noise. Given the read-out noise CKD and the signal value at this stage, we have to divide both components by the number of co-additions. If it is not deemed necessary to have the measurement noise available at the first steps in the reverse model, this is the preferred alternative starting point.

We continue to follow the signal in the reverse model. Note that from now on, the measurement noise is virtual but we want to provide it to the L01b product. Binning gives an extra factor n_{bin}^2 to the noise. Note that one power of n_{bin} vanishes in the shot noise part:

$$S'_{\text{corr-bin}} = \frac{1}{n_{\text{bin}}} S'_{\text{source}} , \quad (36)$$

$$s_{\text{meas}}^2 \{S'_{\text{corr-bin}}\} = \frac{1}{N_{\text{coadd}}} \left(\frac{1}{n_{\text{bin}}} S'_{\text{corr-bin}} + \frac{1}{n_{\text{bin}}^2} \epsilon_{\text{ckd}}^2 \right) . \quad (37)$$

We arrive at the residual correction. Here the signal is joined by some n_{res} residual signals, all having their own measurement noises, also propagated until after the binning correction and the dark current correction. These residual signals are aggregated (see Section 22.8). Their measurement noises are likewise combined:

$$s_{\text{meas}}^2 \{S'_{\text{res,corr-dc}}\} = \frac{1}{n_{\text{res}}^2 N_{\text{coadd}}} \sum_{i=1}^{n_{\text{res}}} \left(\frac{1}{n_{\text{bin}}} S'_{i,\text{res,corr-dc}} + \frac{1}{n_{\text{bin}}^2} \epsilon_{\text{ckd}}^2 \right) . \quad (38)$$

Now we can act in two ways. First, we can consider the residual explicitly as a CKD, with no noise associated. In this formal approach the measurement noise related to the signal itself does not change. Instead, in determining the CKD, the noise is rolled into the error of the CKD and is subsequently propagated as such. This approach will be the baseline.

An alternative approach is to recognize the noise of the residual as proper noise. In that case the measurement noise after the residual correction algorithm step thus yields

$$s_{\text{meas}}^2 \{S'_{\text{corr-res}}\} = \frac{1}{N_{\text{coadd}}} \left[\frac{1}{n_{\text{bin}}} (S'_{\text{corr-dc}} + \frac{1}{n_{\text{res}}} S'_{\text{res,corr-dc}}) + \frac{1}{n_{\text{bin}}^2} \epsilon_{\text{ckd}}^2 (1 + \frac{1}{n_{\text{res}}}) \right] . \quad (39)$$

After that, conversions for exposure time division and to (ir)radiance units follow, giving the virtual measurement noise for the L01b product.

20.4 Effects of binning on signal and variance

All algorithm steps in the reverse model are applied to image pixels. However, pixel-dependent CKD parameters are provided unbinned, while the signal that is to be corrected is binned. The only exception to this rule is residual correction for UVN: residual images are obtained using the same binning as their corresponding illuminated images. The concerned algorithms are PRNU, straylight, slit irregularity and (ir-)radiance responsivity. The binning process in the ROR has two negative effects on the correctness of the model: both the signal itself and its error propagation are affected. These effects are discussed below.

20.4.1 Effect of binning on the signal

Consider a group of N consecutive detector pixels $\mathbf{x}_{\text{det},r}$ on the same column c but different rows r . Then consider that these are binned together into an image pixel \mathbf{x}_{img} . Thus N is the binning factor. Forgetting about the column number c , and writing $r = r_{\text{det}}$ and $R = r_{\text{img}}$, the average binned input signal for the image pixel is expressed in terms of the original input signals of the binned detector pixels as

$$S_i[R] = \frac{1}{N} \sum_r S_i[r] . \quad (40)$$

Note that the individual $S_i[r]$ are not known to the L01b Processor, but for this section, it is assumed that they are. Consider now two hypothetical corrections, one additive and one multiplicative, on this input signal. The additive terms and multiplicative factors for these corrections are available as unbinned calibration key data parameters $c[r]$ and $d[r]$, respectively. To apply these corrections on the binned input signal $S_i[R]$, these CKD parameters have to be binned likewise:

$$c[R] = \frac{1}{N} \sum_r c[r] ; \quad (41a)$$

$$d[R] = \frac{1}{N} \sum_r d[r] . \quad (41b)$$

Now, in the L01b Processor, the additive correction would be implemented as:

$$S_{\text{o,computed}}[R] = S_i[R] + c[R] = \frac{1}{N} \sum_r S_i[r] + \frac{1}{N} \sum_r c[r] . \quad (42)$$

If, however, the correction could be applied before binning,

$$S_{\text{o,true}}[R] = \frac{1}{N} \sum_r (S_i[r] + c[r]) , \quad (43)$$

it is clear that the exact same result is obtained. For the multiplicative correction, however, the computed and true results are not equal. The computed result is:

$$S_{\text{o,computed}}[R] = d[R] S_i[R] = \frac{1}{N^2} \sum_r d[r] \sum_r S_i[r] , \quad (44)$$

while the true result is:

$$S_{\text{o,true}}[R] = \frac{1}{N} \sum_r d[r] S_i[r] . \quad (45)$$

These expressions are equal only if either the $S_i[r]$, the $d[r]$, or both, are constant as a function of row number r . When both the detector signal and CKD parameter have a non-zero gradient as a function of r , this can lead to errors. This can be elaborated on. Note that each of the $d[r]$ are known, but the $S_i[r]$ are not. Write

$$\begin{aligned} S_{\text{o,true}}[R] &= \frac{1}{N} \sum_r d[r] \{S_i[R] + (S_i[r] - S_i[R])\} \\ &= \frac{1}{N} S_i[R] \sum_r d[r] + \frac{1}{N} \sum_r d[r] \{S_i[r] - S_i[R]\} \\ &= S_{\text{o,computed}}[R] + \frac{1}{N} \sum_r d[r] \Delta S_i[r] . \end{aligned} \quad (46)$$

So the error can be described in terms of the deviations $\Delta S_i[r]$. Of course, $\sum_r \Delta S_i[r] = 0$. Although the individual $S_i[r]$ cannot be known, the following can be considered: If the binned signals $S_i[R]$ form a smooth function in the image row direction, it can be expected that this smoothness is propagated on the smaller scale of the detector rows, not taking noise into account, the suppression of which was one of the argued advantages of binning to begin with. This reasoning allows to proclaim the estimates $\widetilde{\Delta S_i[r]}$ for the individual $\Delta S_i[r]$, using interpolating from neighboring binned $S_i[R]$ and the zero summation property. This allows for correcting the computed binned signal as follows:

$$S_{o,corrected}[R] = S_{o,computed}[R] + \frac{1}{N} \sum_r d[r] \widetilde{\Delta S_i[r]} . \quad (47)$$

20.4.2 Effects of binning on error propagation

For the hypothetical additive correction of the previous section, the formal error propagation is

$$\sigma_o^2[R] = \sigma_i^2[R] + s_c^2[R] . \quad (48)$$

A similar equation holds for the multiplicative case. In either case, the not yet defined binned variance $s_c^2[R]$ must be expressed in something meaningful. Assuming that the CKD parameter for two neighboring pixels in the row direction is completely uncorrelated, Bienaymé's formula $\text{Var}(\sum_i X_i) = \sum_i \text{Var}(X_i)$ applies. This gives

$$\sigma_o^2[R] = \sigma_i^2[R] + \frac{1}{N^2} \sum_r s_c^2[r] = \sigma_i^2[R] + \frac{1}{N} \overline{s_c^2[r]} , \quad (49)$$

where the mean variance over the binned rows is defined as

$$\overline{s_c^2[r]} = \frac{1}{N} \sum_r s_c^2[r] . \quad (50)$$

The notation implies that the average is taken over the unbinned detector pixels related to the image pixel under consideration. On the other hand, if the CKD parameter for two neighboring pixels in row direction is completely correlated (for example if the parameter pixels are locally constant), then the general rule applies that the variance of the sum is the sum of their N^2 covariances (including the covariances of pixels with themselves, which are of course the variances).

A special case arises when the unbinned CKD pixels are all equal. Then $s_c^2[R] = \overline{s_c^2[r]}$ to indicate that the variances of the equal unbinned signals can all be substituted with a single binned signal variance. More formally: $\text{Var}(\sum_i X) = \text{Var}(NX) = N^2 \text{Var}X$. (Note that the provided CKD pixels variances can still be different even when the CKD pixels are not!) Now the N^2 in numerator and denominator cancel:

$$\sigma_o^2[R] = \sigma_i^2[R] + s_c^2[R] = \sigma_i^2[R] + \overline{s_c^2[r]} . \quad (51)$$

Note that the mean variance in the second equality is always well-defined. Between these two extremes the propagation formula needs an explicit covariance matrix. If it can be assumed that correlations between different pixels are not negative, the mean binned variance $\overline{s_c^2[r]}$ can be computed, and the differential propagation error is constrained as follows:

$$\frac{1}{N} \overline{s_c^2[r]} \leq \sigma_o^2[R] - \sigma_i^2[R] \leq \overline{s_c^2[r]} . \quad (52)$$

Note, however, that in the case of negative correlations the first inequality does not hold (assume, for example, a bin of size 2 where the second pixel signal correlates exactly oppositely to the first; both variances cancel and the combined variance is then zero).

We now claim that the second inequality always holds, whatever the covariances are, and that we can choose this (i.e. $\sigma_o^2[R] - \sigma_i^2[R] \leq \overline{s_c^2[r]}$) to be the standard strategy in the algorithms concerned. Suppose we have N signals in a bin; we assume first that each signal is completely correlated in some way to the first signal.

$$S[i] = \alpha_i S[1] + \beta_i, \quad 1 \leq i \leq N . \quad (53)$$

Signal $S[i]$ has variance $\sigma^2[i]$. We can relate the variances of the other signals to $\sigma[1]^2$: $\sigma^2[i] = \alpha_i^2 \sigma[1]^2$. Further, the covariance between $S[i]$ and $S[j]$ equals $\sigma[i]\sigma[j] = \sigma[1]^2 \alpha_i \alpha_j$. We can now write the covariance matrix for the completely correlated case as

$$\text{Cov}[S[i], S[j]] = \sigma[1]^2 (\alpha_i \alpha_j) . \quad (54)$$

The binned signal is $S[R] = (1/N) \sum_{i=1}^N S[i]$. Define $A_n = (1/N) \sum_i \sigma^2[i]$ (this is the mean variance $\overline{s_c^2[r]}$) and $B_n = \text{Var} S[R] = (1/N^2) \text{Var} \sum_i S[i] = (1/N^2) \sum_i \sum_j \text{Cov}[S[i], S[j]]$. We want to prove that $A_n \geq B_n$ for all bin sizes N . In the remainder, we omit the scaling factor $\sigma[1]^2$.

We use a proof by induction. Trivially, $A_1 = B_1$. Also, $A_2 - B_2 = \frac{1}{4}(\alpha_1 - \alpha_2)^2 \geq 0$. Assume $A_n - B_n \geq 0$ for some $n > 1$. Then

$$A_{n+1} = \frac{1}{n+1} \sum_{i=1}^{n+1} \alpha_i^2 = \frac{1}{n+1} [nA_n + \alpha_{n+1}^2] \quad (55)$$

and

$$\begin{aligned} B_{n+1} &= \frac{1}{(n+1)^2} \sum_i \sum_j \alpha_i \alpha_j = \frac{1}{(n+1)^2} \left[\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j + 2 \sum_{i=1}^n \alpha_i \alpha_{n+1} + \alpha_{n+1}^2 \right] \\ &= \frac{1}{(n+1)^2} \left[n^2 B_n + 2 \sum_{i=1}^n \alpha_i \alpha_{n+1} + \alpha_{n+1}^2 \right]. \end{aligned} \quad (56)$$

Then

$$\begin{aligned} A_{n+1} - B_{n+1} &= \frac{1}{(n+1)^2} \left[n(n+1)A_n + (n+1)\alpha_{n+1}^2 - n^2 B_n - 2 \sum_{i=1}^n \alpha_i \alpha_{n+1} - \alpha_{n+1}^2 \right] \\ &= \frac{1}{(n+1)^2} \left[n^2(A_n - B_n) + nA_n + n\alpha_{n+1}^2 - 2 \sum_{i=1}^n \alpha_i \alpha_{n+1} \right] \\ &= \frac{1}{(n+1)^2} \left[n^2(A_n - B_n) + \sum_{i=1}^n (\alpha_i^2 + \alpha_{n+1}^2 - 2\alpha_i \alpha_{n+1}) \right] \\ &= \frac{1}{(n+1)^2} \left[n^2(A_n - B_n) + \sum_{i=1}^n (\alpha_i - \alpha_{n+1})^2 \right]. \end{aligned} \quad (57)$$

The first expression between the square brackets is non-negative because of the induction hypothesis, while the second expression is a sum of squares.

If the sequence of individual signals is less than fully correlated, then the off-diagonal entries in the covariance matrix become smaller; this follows easily from $\text{Cov}[S[i], S[j]] = \text{Corr}[S[i], S[j]] \cdot \sigma[i] \cdot \sigma[j]$. In that case, A_n stays the same while B_n decreases.

This ends the proof of the claim that we are allowed to use the mean binned variance $\overline{s_c^2[r]}$ as an upper limit to the error increase. The current descriptions of binned CKD's are consistent with this policy.

21 Generic corrections I

In this section we describe the generic corrections (i.e. valid for both UVN and SWIR) in the beginning of the processing flow, as shown in Figure 46. This first generic set of corrections consists of only one algorithm, namely the co-addition correction.

21.1 Co-addition correction

A number of subsequent images along the flight path has been added in the read-out register. During normal operation, the co-addition factor is expected to be related to the ratio of the ground pixel size and the chosen exposure time. However, the factor is directly set by the engineering data. The maximum allowed co-addition factor is 256. It is wise to not exceed 128 co-additions because if all individual exposures are saturated, their sum will overflow the ICU co-addition buffer.

This algorithm is related to Equation (26) in the forward model part.

21.1.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	DN
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	DN ²
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	DN
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	DN ²
C_{coadd}	co-addition correction factor	1
N_{coadd}	number of co-additions	1

21.1.2 Algorithm description

$$S_o[\mathbf{x}_{img}] = C_{coadd} S_i[\mathbf{x}_{img}], \quad (58)$$

where

$$C_{coadd} = \frac{1}{N_{coadd}}. \quad (59)$$

The signal S_i is the measured signal. It has not yet undergone any correction. Attached to the signal is its error σ_i^2 ; here, at the start of the reverse model, this error is defined to be zero.

21.1.3 Error propagation

$$\sigma_o^2[\mathbf{x}_{img}] = C_{coadd}^2 \sigma_i^2[\mathbf{x}_{img}]. \quad (60)$$

Note that the variance scales with the square of the co-addition factor. This is not an error: In the processor flow, uncertainty propagation is being performed using standard rules, the variance is not computed.

21.1.4 Remark

Clearly, co-addition (in the forward sense) increases the signal-to-noise ratio. Pixels in the small-pixel columns are excluded from this operation. These pixels provide the only way to get some information about changes in a temporal sense during the co-addition time.

Information in the small pixels should be used with caution for the following reasons:

- The noise level of a small pixel is higher than the noise of the co-added pixel. This noise will be broadcast to other pixels, increasing the error of all other signals.
- A column of small pixels is not aligned with one wavelength.
- Pixels outside the small columns have an unknown, and not necessarily positive, correlation with the pixels in the small-pixel columns. The two small-pixel columns themselves are not necessarily correlated with respect to each other. More research is needed to decide on their usage.

22 UVN specific corrections

In the following sections, algorithms that apply only to the UVN modules are described, as shown in Figure 47. These consist of three detectors and account for six spectral bands (Bands 1 through 6).

22.1 Conversion from digital numbers to voltage

In the analog-to-digital converter (ADC) the signal is converted from volts to digital numbers. Therefore, this reverse algorithm multiplies the signal, as measured in digital numbers, with a generic conversion factor (equal for all bands) to arrive at the signal in volts. For consistency reasons, this conversion has been split off from the electronic algorithms (gains and offsets).

This algorithm is related to section 18.3 in the forward model part.

22.1.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	DN
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	DN ²
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	V
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	V ²
f_{dn2v}	unit conversion factor, for all bands	V DN ⁻¹

22.1.2 Algorithm description

$$S_o[\mathbf{x}_{img}] = f_{dn2v} S_i[\mathbf{x}_{img}] , \quad (61)$$

22.1.3 Error propagation

$$\sigma_o^2[\mathbf{x}_{img}] = f_{dn2v}^2 \sigma_i^2[\mathbf{x}_{img}] . \quad (62)$$

The conversion factor is expected to be known exactly; hence its related error term is zero.

There is a caveat here: the digital numbers are, per definition, integers. That means that a rounding procedure has taken place in the forward model. This translates in the reverse model into a quantization error. This error is not measurable since quantization is basically an invertible process. The baseline is to lump the quantization term into the overall read-out noise. This decision is justified by our current estimates of the effective numbers of bits and the read-out noise.

22.2 Electronics gains and offsets

The electronic chain for the UVN detector module consist of a number of components that, combined, give rise to an (additive) electronic offset and a (multiplicative) electronic gain.

The electronic chain consists of three gains and up to four offsets. Three gains and one offset are programmable; in forward order, these are the charge-coupled device (CCD), the correlated double sampler (CDS), the digital-to-analog converter (DAC) offset and the programmable gain amplifier (PGA). The three gains are probably accompanied by their own offsets. We consider the electronic chain as a monolithic block and follow the signal in reverse order.

This algorithm is related to sections 18.2 and 18.3 in the forward model part.

- First, the analog-to-digital converter transforms, in reverse sense, the signal in digital numbers towards volts. This is described in the previous section.
- The PGA gain G_{pga} can be set in 256 steps between $0.7\times$ and $8.0\times$. This gain will introduce an offset O_{pga} , depending on the gain: $O_{pga} = f(G_{pga})$.
- The digital-to-analog converter (DAC) offset O_{dac} can be regarded as quasi-continuous. Its value can vary between -255 mV and 255 mV.
- Then the signal arrives at the CDS. Here, a gain of 1 or 2 must be chosen. Both gains are accompanied by their own offset. This offset may depend on the gain setting, which is denoted by a superscript O_{cds}^L or O_{cds}^H .
- In the analog video chain (AVC), a possible offset can be introduced. This does not matter, since the AVC gain is fixed and the introduced offset is expected to remain constant. The video amplifier always contributes an *absolute* gain factor; this gain does not depend on the chosen gain settings. For this AVC gain G_{abs} the designer setting is taken.
- Finally, the CCD gain setting G_{ccd} . An offset $O_{ccdbias}$ is introduced during this conversion. This offset may depend on the gain setting, which is denoted by a superscript ($O_{ccdbias}^L$ or $O_{ccdbias}^H$).

The gains and offsets are combined in one system gain and one system offset; both are calibration key data.

The *measured* signal has an offset O_{sys} . The difference between the electronic offset and the total (system) offset is the detector offset: $O_{\text{detector}} = O_{\text{sys}} - O_{\text{elec}}$. This quantity consists of smear and other terms; only the smear remains after a background subtraction operation. We therefore have to stress that the offset to be corrected for in this algorithm step is only the electronic offset.

For the gains, no difference between measured and electronic gain exist and we can write $G_{\text{sys}} = G_{\text{elec}} = G_{\text{abs}} \cdot G_{\text{rel}}$. Note that the analog video amplifier contribution is expressed by a given quantity G_{abs} : without loss of generality, we can set it to the design value. The gain proper G_{rel} is relative; that is, for the reference gain setting \mathbf{g}_{ref} , the relative gain G_{rel} equals one.

Since the process above in the forward model is described as $S_{\text{after}} = G_{\text{sys}}S_{\text{before}} + O_{\text{elec}}$, the algorithm step in the reverse model should implement the inverse formula.

22.2.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	V
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	V ²
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	V
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	V ²
G_{sys}	total system gain, per band	1
O_{sys}	system offset, per band	V
O_{elec}	electronic offset, per band	V
G_{abs}	absolute gain introduced by the video amplifier	V
G_{rel}	total system gain ratio, per band	1
G_{abs}	absolute gain from AVC	1
\mathbf{g}	gain settings code, consisting of three individual settings	1
\mathbf{g}^*	gain and offset settings code, consisting of a 4-tuple of \mathbf{g} and DAC setting.	1
μ	mean signal of the overscan pixel	V
$S[\mathbf{x}_{\text{os}}]$	signal in overscan pixel \mathbf{x}_{os}	V
n_{os}	number of overscan pixels	1
s_{os}^2	variance of an overscan pixel	V ²
s_{μ}^2	mean variance of overscan pixels	V ²
s_{gain}^2	variance of G_{sys}	V ²
$\sigma_{\text{offset}}^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after offset correction only	V ²

22.2.2 Algorithm description

The correction step is

$$S_o[\mathbf{x}_{\text{img}}] = \frac{S_i[\mathbf{x}_{\text{img}}] - O_{\text{elec}}}{G_{\text{sys}}} . \quad (63)$$

This formula is the combined expression of a gain division after an offset subtraction. The gain and offset are defined for all pixels of the band. Dependencies on rows, columns or both, if present, will be dealt with elsewhere. The formula is applied to all pixels, including small-pixel data.

22.2.3 Error propagation

For clarity, we divide the error propagation in two sequential parts: first the offset correction, then the gain correction.

The offset CKD is the result of a measurement that is independent of the current – or of any – signal. The computed offset is the mean $\mu = \overline{S[\mathbf{x}_{\text{os}}]}$ of n_{os} individual overscan pixels. Therefore, the standard computational rules apply. The unbiased estimator of the standard deviation is

$$s_{\text{os}}^2 = \frac{1}{n_{\text{os}} - 1} \sum_{\mathbf{x}_{\text{os}}} (S[\mathbf{x}_{\text{os}}] - \mu)^2 , \quad (64)$$

while the variance of the mean offset is

$$s_{\mu}^2 = \frac{1}{n_{\text{os}}(n_{\text{os}} - 1)} \sum_{\mathbf{x}_{\text{os}}} (S[\mathbf{x}_{\text{os}}] - \mu)^2. \quad (65)$$

The propagation of the offset part is therefore:

$$\sigma_{\text{offset}}^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] + s_{\mu}^2. \quad (66)$$

The gain CKD is the result of an elaborate procedure. However, the baseline procedure consists of taking the ratio of the averages of all individual pixel regression line slopes. The calibration measurements were not suitable for invoking Eq. 43 (concerning error propagation of inverse calibrated quantities) in the scientific quality requirements document (see [AD3]). Instead, we assume a variance CKD of the gain ratio s_{gain}^2 . The propagation of the gain part is therefore:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \frac{1}{G_{\text{sys}}^2} \sigma_{\text{offset}}^2[\mathbf{x}_{\text{img}}] + \frac{s_{\text{gain}}^2}{G_{\text{sys}}^4} (S_i[\mathbf{x}_{\text{img}}] - O_{\text{elec}})^2. \quad (67)$$

This gives for the combined error propagation for both offset and gain:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \frac{1}{G_{\text{sys}}^2} (\sigma_i[\mathbf{x}_{\text{img}}]^2 + s_{\mu}^2) + \frac{s_{\text{gain}}^2}{G_{\text{sys}}^4} (S_i[\mathbf{x}_{\text{img}}] - O_{\text{elec}})^2. \quad (68)$$

22.2.4 Dynamic offset correction

The above propagation algorithms assume that the offset, and its error, are available as CKD parameters. These parameters are therefore *static*. In addition, the offset may be determined *dynamically* from parts of the image that contain no actual signal apart from that induced by the electronic components mentioned above.

This leads to several types of offset values that may be used in formulas above: static, dynamically from overscan columns, dynamically from pre- and postscan columns, dynamically from overscan rows, and dynamically from the read-out register. Note that the ROR employs only one of the CCD gain settings. Therefore, this method will only yield electronic dynamic offsets for that CCD gain setting.

Each dynamic method uses its own number of suitable pixels n_{os} and region \mathbf{x}_{os} in the formulas 64 and 65. Note that the amount of pixels involved will in general be much smaller than for the dedicated CKD measurements; therefore, the associated error of the dynamic offset will be larger. On the other hand, dynamically determined offsets can be highly accurate in the sense that they are measured at the same time as the signal; unmodeled effects such as drifts (compared to the circumstances during calibration) are then automatically taken into account.

22.2.5 Remarks

In the algorithm, we did not perform the unit conversions from DN to volts to electrons as suggested by the description of the electronic chain. So, although in the processing algorithm, the whole electronic chain is treated as one block, we have chosen to separate both conversions from the gain and offset algorithm step. The rationale is that other conversions are also performed in their own algorithm step. Conversion between these units is straightforward, however, so this choice will not be more cumbersome than others.

The offset correction is the same for each pixel. It is therefore possible that an individual pixel signal still contains some electronic offset. We can use the acronym PONU (Pixel offset non-uniformity) for this offset.

We will now briefly discuss if PONU has more than merely theoretical impact. First, a pixel offset should not be confused with read-out noise. A sufficient signal-to-noise ratio is needed to check for that. PONU can be defined as the intercept of a signal, generated by constant light flux, defined at several exposure times, but after having taken the correction for smear into account. The only other correction step before the exposure time division (at which stage the signal should definitely be modeled as a flux times exposure time) is the residual correction. This residual is defined per ICID. It can contain unmodeled artifacts like EMC. A residual for zero exposure time cannot be defined. However, we can define PONU as a constant common part of all residual ICIDs of which all settings, except for the exposure time, are identical. But this definition is merely academic. In any case, after the residual correction any electronic offset has per definition disappeared. PONU, if it is nonzero, will only exist between the offset correction and residual correction. No algorithm, whether in the L01b Processor or the calibration algorithm, is influenced by its possible existence.

22.3 Conversion from voltage to charge

In the CCD part of the electronic chain, the signal in forward direction is converted from charge to voltage. Therefore, in the reverse model, the inverse conversion takes place. The conversion, however, is not entirely linear as function of the signal. This non-linear behavior will be separately addressed, and corrected for, in the next section.

This algorithm is related to Section 18.1 in the forward model part.

22.3.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	V
$\sigma_1^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	V ²
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	e ⁻
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e ⁻²
f_{v2e}	unit conversion factor, per band	e ⁻ V ⁻¹

22.3.2 Algorithm description

$$S_o[\mathbf{x}_{img}] = f_{v2e} S_i[\mathbf{x}_{img}] , \quad (69)$$

22.3.3 Error propagation

$$\sigma_o^2[\mathbf{x}_{img}] = f_{v2e}^2 \sigma_1^2[\mathbf{x}_{img}] . \quad (70)$$

The conversion factor is expected to be known exactly. However, the exact factor will be an adjustment of the design value. This adjustment stems from calibration measurements; it will ensure that a signal measured on a detector, expressed in electrons, will be continuous on both sides of the inter-band boundary. The notion of an error is meaningless since such a discrepancy is completely correlated to the PRNU CKD error. Hence we define the error term of the conversion factor to be zero.

22.4 Non-linearity correction

The voltage-to-charge conversion algorithm performs two actions. The first, mentioned in the previous section, is a straightforward unit conversion, the second a more elaborate correction for the CCD non-linearity. The non-linearity stems from the charge-to-voltage conversion at each CCD output node. It is, by construction, the same for all pixels.

For each band and for both CCD gain settings the non-linearity is determined in the following way: LED measurements for a range of exposure times are performed such that the highest exposure times result in up to 100% register full well, while the lower exposure times show a linear behavior of the register charge as function of the exposure time. Ideally, the latter measurements coincide with the gain ratio calibration measurements. The non-linearity is now defined as the difference between the expected linear behavior and the actually measured register charges. This difference is then converted to a function of the measured signal, instead of the exposure time. More information can be found in [RD11].

The derived non-linearity curves and their uncertainties are CKD parameters. Per construction and per definition, the non-linearity is zero for the zero signal. If not, an extra offset would be introduced in the correction.

This algorithm is related to Section 18.1 in the forward model part.

22.4.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$e^{-,2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$e^{-,2}$
$f_{\text{ccd}}(S_i[\mathbf{x}_{\text{img}}])$	non-linearity correction function, per band	e^- / e^-
$s_{\text{ckd}}^2(S_i[\mathbf{x}_{\text{img}}])$	variance of the non-linearity correction function	$e^{-,2}$
$s_{\text{noise}}^2(S_i[\mathbf{x}_{\text{img}}])$	noise part of the non-linearity error	$e^{-,2}$
$s_{\text{ccd}}(S_i[\mathbf{x}_{\text{img}}])$	envelope of the calibration measurements for the non-linearity function	e^-
L_{max}	upper limit of linear range for read-out values	e^-
L_{sat}	saturation threshold, related to register full well	e^-
N	order of the pynomials describing non-linearity and its error	1
$s_{\text{coadd}}^2[\mathbf{x}_{\text{img}}]$	variance due to co-additions	$e^{-,2}$

22.4.2 Algorithm description

A polynomial function f_{ccd} is evaluated for the measured pixel signal; the outcome is subtracted from the signal.

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] - f_{\text{ccd}}(S_i[\mathbf{x}_{\text{img}}]) . \quad (71)$$

We expect all signals with low charges to behave as a linear function of the corrected exposure time. More specific, we define the line describing this behavior by two points, associated with zero charge and a predefined charge L_{max} . The choice for L_{max} depends on the expected behavior of the CCD and must be the same for all pixels.

The non-linearity function f_{ccd} can be rather complicated. Its definition depends on the input value S_i . We have $f_{\text{ccd}}(0) = 0$ and $f_{\text{ccd}}(L_{\text{max}}) = 0$. Further, it is expected that f_{ccd} is small, in absolute sense, for charges in the interval $(0, L_{\text{max}})$. Above the saturation threshold L_{sat} , which is related to the register full-well, the polynomial regression fit no longer holds and the function is undefined. Below the L_{sat} threshold, the non-linearity is described using a Chebyshev polynomial of a certain order N . The corresponding $N + 1$ Chebyshev coefficients, together with the two threshold values, are sufficient to evaluate the function.

22.4.3 Error propagation

The non-linearity function $f_{\text{ccd}}(Q)$ can be regarded as the mean correction term for a certain charge Q . Likewise, an accompanying function $s_{\text{ckd}}(Q)$ denotes the standard deviation of the correction term for the same Q . That is, both the non-linearity correction and its standard deviation/variance depend on the value of the signal S_i .

We addressed some difficulties in establishing the variance of the calibration key data already in the aforementioned document [RD11]. The total CKD error is constituted of three terms: The inherited L01b Processor error s_{01b}^2 , the error stemming from the noise s_{noise}^2 and the error in the polynomial approximation s_{curve}^2 of the actual, albeit unknown, function. These three terms are defined as a function of signal S_i instead of pixel \mathbf{x}_{img} . After adding these three terms, this total error is again described with a Chebyshev polynomial, on the same interval as the non-linearity function itself. Note that we could, in principle, recursively define a curve error of the polynomial expansion of the error, but then we would try to model second-order effects. We discuss three aspects of the error: The noise part of the CKD error, the implementation of the propagation, and the role of co-additions.

First, the **noise part of the CKD error**. In order to model the error stemming from the noise, we first consider the simplified case of linear regression. Note that, in the case of linear regression instead of Chebyshev polynomial regression with order N , the variance would be like:

$$s_{\text{lin}}^2(S_i[\mathbf{x}_{\text{img}}]) = s_{\text{ccd}}^2(S_i[\mathbf{x}_{\text{img}}]) \left(1 + \frac{1}{n_{\text{ref}}} + \frac{(S_i[\mathbf{x}_{\text{img}}] - \bar{X}_{\text{ref}})^2}{S_{\text{XX,ref}}} \right) . \quad (72)$$

We argue that the first term 1 is to be dropped since we are not performing individual observations with measurement noise here and therefore only consider the mean value of the non-linearity function. Here a few

ancillary symbols are introduced: n_{ref} denotes the number of observations involved in the linear part of the calibration, \bar{X}_{ref} denotes the mean of the signal observations in the linear part of the calibration, and $S_{XX,\text{ref}}$ denotes the sum of squared deviations from the mean $\sum_i (X_i - \bar{X}_{\text{ref}})^2$. The subscript ‘ref’ is a reminder that the non-linearity calibration measurements have been performed with the reference gain, in order for them to be compared with the gain ratio calibration measurements.

Now, we move on to the actual case of higher order regression. Clearly, the standard deviation of an individual measurement is $s_{\text{ccd}}(Q)$ as obtained during the computation of the CKD. Graphically, it is the width of the envelope around the cloudy function to be parametrized by the Chebyshev polynomial f_{ccd} .

We would like to use a variant of Equation (72) that works for higher orders. The third term of the equation, invoking the pivoting of the slope around \bar{X} is now meaningless since there is no longer a slope coefficient with global influence. Instead, we should recognize the localized character of the regression curve and change the variable n_{ref} into a localized definition: $n_{\text{ref}} = n_{\text{obs}}/N$ where N is the order of the polynomial describing the curve. To state the matter loosely, we expect that per Chebyshev node only the nearby surrounding observations are important. Therefore:

$$s_{\text{noise}}^2(S_i[\mathbf{x}_{\text{img}}]) = s_{\text{ccd}}^2(S_i[\mathbf{x}_{\text{img}}]) \left(0 + \frac{N}{n_{\text{obs}}}\right), \quad (73)$$

where we again discard the first term 1 as being the instrumental error.

Another possibility is that the said envelope is persistent, i.e. does not become thinner when the noise is decreased. This can be the case if instrument behavior remains outside a model, for example an unknown additional non-linearity. In that case s_{noise}^2 must be replaced by s_{ccd}^2 . This gives the CKD error as obtained from on-ground calibration:

$$s_{\text{ckd}}^2[S_i] = s_{\text{i01b}}^2[S_i] + s_{\text{noise}}^2[S_i] + s_{\text{curve}}^2[S_i]. \quad (74)$$

Then, the **implementation of the error propagation**. The signal is propagated as $S_o = S_i - f_{\text{ccd}}(S_i)$. Formally, we can write the error propagation of a function $g(S_i) = S_i - f(S_i)$ as

$$s_g^2 = \left(1 - \frac{df_{\text{ccd}}}{dS_i}\right)^2 s_{S_i}^2 = \left(1 - \frac{df_{\text{ccd}}}{dS_i}\right)^2 \sigma_i^2. \quad (75)$$

However, we have to take into account that f_{ccd} is not known exactly: it has its own error $s_{f,\text{ccd}}^2$, in this case given by the available CKD function s_{ckd}^2 . We cannot formalize this but instead choose a pragmatic solution: this error serves as an extra additive term. (Alternatively, we can write $g = g(S_i, f)$ and error propagation gives an extra term $(dg/df)^2 s_f^2 = (-1)^2 s_{\text{ckd}}^2$. This seems to work well, although the correlation between S_i and f is hard to define.) Note further that, although we can write $f_{\text{ccd}} = \sum c_j T_j$, we are not allowed to perform formal error propagation using $g = g(S_i, c_0, \dots, c_N)$ since the c_j are correlated. Therefore we state that the error propagation formula is

$$\sigma_o^2 = \left(1 - \frac{df_{\text{ccd}}}{dS_i}\right)^2 \sigma_i^2 + s_{\text{ckd}}^2. \quad (76)$$

Equation (76) makes it necessary to evaluate not only the non-linearity function itself, but also its derivative, expressed in Chebyshev polynomials. Fortunately, the derivative of a Chebyshev polynomial expression is easily computed, see Appendix A.

Finally, we discuss the **role of co-additions**. We make an error because we are correcting the co-added signal instead of the individual original signals. This is a second-order effect. It is difficult to get an indication of the size of the error since we do not have the original signals of each frame. However, we can make use of the small-pixel columns to get a rough estimation. In case of co-addition, any signal S is the mean of N_{coadd} frame signals $S_{\text{coadd},j}$. So we make the following error, where we use the shorthand notation S as argument for the non-linearity function:

$$\sigma_{\text{coadd}}^2 = \left[f_{\text{ccd}}(S) - \frac{1}{N_{\text{coadd}}} \sum_{j=1}^{N_{\text{coadd}}} f_{\text{ccd}}(S_{\text{coadd},j}) \right]^2. \quad (77)$$

We repeat that we do not know the original $S_{\text{coadd},j}$. Instead we make an estimate by using scaling factors based on the small-pixel data:

$$s_{\text{coadd}}^2 = \left[f_{\text{ccd}}(S) - \frac{1}{N_{\text{coadd}}} \sum_{j=1}^{N_{\text{coadd}}} f_{\text{ccd}}(\alpha_j S) \right]^2. \quad (78)$$

Here the α_j give an estimate of the temporal change of the entire image, based on the two small-pixel columns, such that $\sum_{j=1}^{N_{\text{coadd}}} \alpha_j = N_{\text{coadd}}$. If this estimate cannot be made, we can as a worst-case scenario choose the set

of α_j and therefore the non-linearities $f_{ccd}(\alpha_j S)$ such that the deviations are largest. The total error propagation is now

$$\sigma_o^2[\mathbf{x}_{img}] = \left(1 - \frac{df_{ccd}}{dS_i}(S_i[\mathbf{x}_{img}])\right)^2 \sigma_i^2[\mathbf{x}_{img}] + s_{ckd}^2(S_i[\mathbf{x}_{img}]) + s_{coadd}^2[\mathbf{x}_{img}]. \quad (79)$$

22.5 Read-out register binning correction

In the read-out register of the CCD, a number of rows has been binned. That integer number is called the binning factor; it can vary per band or across the detector in the row direction. As a consequence, individual CCD pixel signals have been lost; only their sum is known. The disadvantage of the loss of information is counterbalanced by the increased signal-to-noise ratio. This algorithm is related to Section 17.2.1 in the forward model part.

22.5.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
$n_{bin}[r_{img}]$	binning factor related to the current image row	1

22.5.2 Algorithm description

The binning factor can be determined from the binning table. The binning table is an attribute of the measurement; per image row, it gives the number of corresponding detector rows $n_{bin}[r_{img}]$, also known as the binning factor, and, indirectly, of the detector row numbers. The transformation function becomes:

$$S_o[\mathbf{x}_{img}] = \frac{S_i[\mathbf{x}_{img}]}{n_{bin}[r_{img}]} . \quad (80)$$

22.5.3 Error propagation

$$\sigma_o^2[\mathbf{x}_{img}] = \frac{\sigma_i^2[\mathbf{x}_{img}]}{n_{bin}^2[r_{img}]} . \quad (81)$$

Note that the variance scales with the square of the binning factor. This is not an error: In the processor flow, we are merely performing uncertainty propagation using the standard rule: $\text{Var}(aX) = a^2\text{Var}(X)$.

22.6 Charge transfer efficiency

Charge transfer has two effects on the signal: The first is that during each transfer the amount of charge is multiplied by the efficiency, which results in a loss of charge. The second is that the pixel to which the charge is transferred is not empty but has the residual from the previous charge. This is effectively a charge addition. Charge transfer is clearly a conservative process and for a homogeneous illumination the loss and addition cancel out. For inhomogeneous illumination, the total residual effect is a slight smearing of the signal. Other charge transfer effects are expected to be very small in TROPOMI because the signal levels are such that dislocations are continuously in a filled state.

This algorithm is related to Section 17.2 in the forward model part.

22.6.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
\mathbf{A}	pixel response matrix	1
\mathbf{A}_{hor}	pixel response matrix for horizontal transfers in ROR	1
\mathbf{A}_{vert}	pixel response matrix for vertical parallel transfers	1
$S_n[r]$	Signal from position r after N transfers	e^-
$\varepsilon[\mathbf{x}_{\text{det}}]$	Charge transfer inefficiency	1
$n_{\text{rows,image}}$	Number of detector rows in the image section	1
$n_{\text{rows,storage}}$	Number of detector rows in the storage section	1
n_{cols}	Number of detector columns	1
n_{rows}	Total number of detector columns including storage section and ROR	1
σ_{cte}^2	Extra signal variance introduced by CTE	e^{-2}

22.6.2 Algorithm description: theory

If the charge transfer efficiency (CTE) of each pixel location is known, the combined effect of all vertical and horizontal transfers can be modeled using a pixel response matrix \mathbf{A} . The idea is the following. All pixels $[r_{\text{det}}, c_{\text{det}}]$ are numbered in reading order; the value of A_{ij} denotes the fraction of the charge originally located in pixel j that ends up in pixel i .

The matrix most probably is quite diagonally dominant; if there is no charge transfer inefficiency, \mathbf{A} is the identity matrix. Otherwise, charges originally located in neighboring pixel locations downstream will change the signal, though the contribution of pixels farther away will decrease fast. Further, if pixel i is downstream (i.e. has a lower row number) of pixel j then $A_{ij} = 0$: pixel j does not influence pixel i . Another property is that the sum of each column of \mathbf{A} equals one.

\mathbf{A} is a large square matrix with $(n_{\text{rows,image}} + n_{\text{rows,storage}} + 1) \times n_{\text{cols}}$ rows. Both the rows in the image section and in the storage section have to be counted, while the ROR gives an extra row. n_{cols} is the number of CCD columns. \mathbf{A} is applied to a column vector containing all pixel and ROR charges. This matrix is too large for practical purposes. Fortunately, most pixels do not interact with each other. For example, during the parallel row transfer pixel charges in the same row have no correlation.

We construct therefore two much smaller response matrices that perform the same task: A matrix \mathbf{A}_{hor} containing $n_{\text{cols}}/2$ rows and a matrix \mathbf{A}_{vert} containing $n_{\text{rows}} = n_{\text{rows,image}} + n_{\text{rows,storage}} + 1$ rows. Both matrices are again square. \mathbf{A}_{hor} handles the horizontal transport in the ROR. Since there are two output nodes per detector (i.e. one per band), only half the number of detector columns are needed in this matrix. \mathbf{A}_{vert} handles the vertical transport of parallel row transfers through the image section and the storage section towards the ROR.

We will now explicitly derive the vertical transfer part of the matrix; the horizontal transfer is similar. Consider a series of vertical transfers with a constant pixel charge transfer inefficiency (CTI) ε for all pixels in the column. Further, $S_n[r]$ denotes the signal at original detector row number r after n row transfers. Thus the wanted (original) signal at the end of the exposure time is $S_0[r]$; after n row transfers, the parcel with electrons obtained at pixel r has arrived at pixel $r - n$. After $n = r$ transfers, the parcel has arrived in the storage area; after $n = r + n_{\text{rows,storage}}$ transfers, the parcel is in the ROR.

Both the positive and negative effects of CTE on the charge are described by

$$S_{n+1}[k] = (1 - \varepsilon)S_n[k] + \varepsilon S_n[k - 1] . \quad (82)$$

So the first few row transfers give

$$S_1[k] = (1 - \varepsilon)S_0[k] + \varepsilon S_0[k - 1]; \quad (83a)$$

$$\begin{aligned} S_2[k] &= (1 - \varepsilon)S_1[k] + \varepsilon S_1[k - 1] \\ &= (1 - \varepsilon)^2 S_0[k] + 2(1 - \varepsilon)\varepsilon S_0[k - 1] + \varepsilon^2 S_0[k - 2]; \end{aligned} \quad (83b)$$

$$S_2[k - 1] = (1 - \varepsilon)^2 S_0[k - 1] + 2(1 - \varepsilon)\varepsilon S_0[k - 2] + \varepsilon^2 S_0[k - 3]; \quad (83c)$$

$$\begin{aligned} S_3[k] &= (1 - \varepsilon)S_2[k] + \varepsilon S_2[k - 1] \\ &= (1 - \varepsilon)^3 S_0[k] + 3\varepsilon(1 - \varepsilon)^2 S_0[k - 1] + 3\varepsilon^2(1 - \varepsilon)S_0[k - 2] + \varepsilon^3 S_0[k - 3] \end{aligned} \quad (83d)$$

and so on according to the binomial series. It is clear that contributions from lower rows become increasingly small due to the powers of ε in the coefficients. The pixel response matrix entries in a matrix row k are precisely the coefficients above after all row transfers: in matrix column j (where $j \leq k$) the coefficient for $S_0[k - j]$ is set:

$$A_{\text{vert},kj} = \binom{k + n_{\text{storage}}}{j + n_{\text{storage}}} (1 - \varepsilon)^{j + n_{\text{rows},\text{storage}}} \varepsilon^{k-j}. \quad (84)$$

Note we can lump the entries for $j \ll k$ to zero without penalty. Thus \mathbf{A}_{vert} is lower diagonal with a small number of non-zero diagonal bands. The total charge transfer effect is computed by

$$\mathbf{S}_{\text{CTE}}[r_{\text{det}}^+] = \mathbf{A}_{\text{vert}} \mathbf{S}_0[r_{\text{det}}^+], \quad (85)$$

where r_{det}^+ is shorthand for all detector pixels including the pixels in the storage area. Note that $\mathbf{S}_{\text{CTE}}[r_{\text{det}}^+]$ are the measured signals, of which we know that the image section part contains the $S_i[r_{\text{det}}]$. The charge transfer efficiency algorithm reverses the process by applying the inverse of the matrix:

$$\mathbf{S}_0[r_{\text{det}}^+] = \mathbf{A}_{\text{vert}}^{-1} \mathbf{S}_{\text{CTE}}[r_{\text{det}}^+]. \quad (86)$$

We only need the lower halves of the vector \mathbf{S}_0 and of the inverse matrix since the upper halves contain signals in the storage area of the detector, in which we are not interested. Note that, although all pixels in the same detector row are transferred in parallel, the matrix is not necessarily the same for each column signal.

We can in a similar way derive the horizontal transfer part of the matrix. Note that the matrix rows resemble wavelength, and the transition described by the matrix shifts charges from one wavelength pixel to another. This effect will be larger for columns halfway the CCD, since their charge parcels travel the largest distance to their assigned output node.

In order to complete the description of the CTE correction algorithm we have to address the following aspects:

- The vertical matrix should be reduced to a binned one.
- The CTE need not to be constant.
- Artefacts like dead pixels and charge sinks.
- We need a combined formula for the matrix product for the horizontal and vertical transfers.

It is currently not baseline to correct for charge transfer inefficiency, therefore it is $\mathbf{A} = \mathbf{I}$. In case a CTI correction becomes necessary at a later stage, the aspects above need to be considered.

22.6.3 Algorithm description: practice

The baseline is that CTE is not modeled, hence the matrix \mathbf{A} is the identity matrix:

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}]. \quad (87)$$

22.6.4 Error propagation

If we do not model the CTE, we make an error depending on the original (i.e. before transfers) charge field. We consider two worst-case scenarios.

Positive spike First, suppose that all pixels of the CCD are completely empty, and a pixel at position $(n_{\text{rows}}, n_{\text{cols}}/2)$ is injected with a signal S_H . The charge transfer inefficiency is ε for all pixels. Then no charge will be added, and at each transfer a fraction $(1 - \varepsilon)$ of the signal is kept. After all parallel and serial transfers, we have at the read-out node

$$S_{H,\text{CTE}} = (1 - \varepsilon)^{n_{\text{rows}} + n_{\text{cols}}/2} S_0 \approx 0.987 S_H, \quad (88)$$

assuming that $\varepsilon = 5 \times 10^{-6}$.

Negative spike Then, for another scenario, consider a large signal gradient in the row direction, with a low signal S_L on the top row and a high signal S_H on all other rows. Then the low signal will mostly acquire charges along its way to the ROR. The amount of signal it picks up is, in first-order approximation, the amount of signal that S_H on the row below does not retain:

$$S_{L,\text{CTE}} \approx (1 - (1 - \varepsilon)^{n_{\text{rows}} + n_{\text{cols}}/2}) S_H + S_L. \quad (89)$$

Using the same approximation for ε and a ratio between the high and low signal of 15, the diffusive effect increases the low signal with 20%.

We can without loss of generality put the error effects in a general error term s_{CTE}^2 that can depend on other pixels, as the scenarios above show:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] + s_{\text{CTE}}^2. \quad (90)$$

It is currently not baseline to correct for charge transfer inefficiency, therefore this error term can be discarded. Any diffusive effects that are present are being handled with in other processing steps like PRNU and straylight.

22.7 Dark current correction

Apart from the actual illuminating signal, the signal recorded by the CCDs consists of a number of additional components. These components, all additive, need to be corrected for in the L01b Processor. We have already discussed the electronic offset (Section 22.2); other components are residual (Sections 22.8 and 22.9) and smear (Section 22.10).

Measurements without illumination, the so-called background measurements, contain only a few of these additive components. At this stage in the L01b Processor, with the offset already having been coped with, the background images contain dark current, electromagnetic compatibility (EMC) and, depending on its definition, pixel-to-pixel offset non-uniformity (PONU).

One strategy is to treat these three terms together. We suppose that for every instrument configuration, a dual, but dark, image of the illuminated image under consideration is provided. Such an image is taken as close in time as possible as the associated illuminated signal. Thus, all instrument settings are the same as for the corresponding illuminated images, except for the presence of the light source. This background image, possibly an aggregate, and containing precisely the three offset terms (dark current, EMC and PONU), can then be subtracted from the actual illuminated signal.

We do not follow that strategy. Instead, the dark current part can be separately determined by calibration measurements. The present algorithm performs the dark current correction using this dark current CKD. What remains of the additional components is called the residual signal. By construction, a background signal with the dark current component removed contains only the residual signal. An illuminated signal will be subjected to the residual correction in the residual correction algorithm, see Section 22.9. Trivially, a background signal corrected for dark current and subsequently for the residual signal becomes the zero signal.

This algorithm is related to Section 17.1 in the forward model part.

22.7.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
T	Temperature	K
T_{ref}	Reference temperature	K
$f_{\text{dc,image},T_{\text{ref}}}[\mathbf{x}_{\text{det}}]$	dark current CKD, image section part	e^-s^{-1}
$f_{\text{dc,storage},T_{\text{ref}}}[c_{\text{det}}]$	dark current CKD, storage section part	e^-s^{-1}
$s_{\text{dc,image},T_{\text{ref}}}^2[\mathbf{x}_{\text{det}}]$	variance of image section dark current CKD	$e^{-2}s^{-2}$
$s_{\text{dc,storage},T_{\text{ref}}}^2[c_{\text{det}}]$	variance of storage section dark current CKD	$e^{-2}s^{-2}$
$S_{\text{dc}}[\mathbf{x}_{\text{det}}]$	dark current part of signal	e^-
t_{exp}	exposure time, including frametransfer time	s
$t_{\text{storage}}[r_{\text{img}}]$	residence time of pixel in storage section	s
$g(T, T_{\text{ref}})$	temperature dependency of dark current, per band	1
$s_g^2(T, T_{\text{ref}})$	variance of temperature dependency of dark current, per band	1

22.7.2 Algorithm description

In section 17.2.1, the six stages of the charge life cycle are described. During each stage, a pixel accumulates some dark current. However, it is cumbersome to model the dark current increase of the complete life cycle.

We have to keep the following in mind:

- Each physical location on the detector, both in the image section and on the storage section, generates an individual amount of dark current; therefore, the dark current is pixel-dependent.
- Dark current is strongly dependent on the (detector) temperature; more than any other electronic contribution (like electronic offset). Therefore we need a relation g that describes the dark current at a certain temperature compared to a reference temperature (being the temperature associated with the dark current CKD measurements). This temperature dependency holds for an entire detector and is therefore not pixel-dependent.

A perfect model would describe the amount of dark current as $\int_{\text{life cycle}} f_{\text{dc}}(x(t)) dt$: the infinitesimal sum of the dark current, at the specific location of the charge, at each time interval. We now assess the aspects of the charge life cycle that will lead to an *approximate* model:

- The 'proper' dark current is generated while the charge resides at its nominal location in the image region. This charge is added to the the electrons generated from photons of the light source. This contribution is $\int_{t_1}^{t_2} f_{\text{dc,image}}[\mathbf{x}_{\text{det}}] dt = f_{\text{dc,image}}[\mathbf{x}_{\text{det}}] \cdot (t_{\text{exp}} - t_{\text{frametransfer}})$.
- During the frame transfer in the image area, the charge accumulates dark current from each pixel in its column, before the exposure between t_0 and t_1 ; after the exposure between t_2 and t_3 . This is 'dark current image smear'. It is expected that relative variations in dark current flux in a column will be small (an assumption that obviously does not hold in the case of 'standard' illumination smear). However, without making the algorithm more complex we can model this contribution exactly using the average per column: $\frac{t_{\text{frametransfer}}}{n_{\text{rows}}} \sum_{r'} f_{\text{dc,image}}[r', c]$. The column average is provided as CKD.
- The amount of time that a charge spends in the storage section is dominated by the limited speed of the read-out: the ADC reads a single pixel in $1/f_{\text{adc}}$ seconds, where $f_{\text{adc}} = 5\text{ MHz}$. That means, for example, that the pixel nearest to the read-out node of an unbinned image resides 0.1 seconds shorter in the storage area than a diametrically opposed pixel in the highest row. This difference clearly needs to be modeled. The actual process, taking binning into account, is more intricate and is described in section 9.1.4. This section also contains the exact calculation of t_{storage} .

- The storage region dark current flux can in principle be measured for each storage pixel location. However, because of the non-trivial chain of movements and residences of a charge in the storage area, a column-dependent value for the storage section dark current flux $f_{dc,storage}[c_{img}]$ is imposed. This value, multiplied with the storage section residence time, determines the storage section dark current.
- Some dark current is generated during the serial transfer in the lowest row in the storage section, between t_5 and t_6 . This dark current can immediately be provided by a CKD as $S_{dc,serial}[c_{img}]$, although also an explicit linear model can be envisaged here.
- Note that the storage section dark current can be regarded as an ICID-dependent offset: while defining the image section dark current as the slope of a graph resulting from background measurements at two different exposure times, the intercept of the connecting line indicates the dark current that both measurements share: the storage section dark current *provided that all other offsets have accurately been removed beforehand*.

To summarize, we model the dark current as the sum of image section dark current and storage section dark current:

$$S_{dc}(T, t_{exp})[\mathbf{x}_{img}] = (A + B + C + D) \cdot g(T, T_{ref}); \quad (91)$$

$$A = f_{dc,image,T_{ref}}[\mathbf{x}_{det}] \cdot (t_{exp} - t_{frametransfer}); \quad (92)$$

$$B = \frac{1}{n_{rows}} \left(\sum_{r'} f_{dc,image,T_{ref}}[r', c_{img}] \right) \cdot t_{frametransfer}; \quad (93)$$

$$C = f_{dc,storage,T_{ref}}[c_{img}] \cdot t_{storage}[r_{img}]; \quad (94)$$

$$D = S_{dc,serial}[c_{img}] = \alpha_1 c_{img} + \alpha_2. \quad (95)$$

Since we can claim that the term D will be very small for in-flight situations, we will omit D and its error s_d^2 in the L01b Processor.

We now elaborate on the temperature relation $g(T, T_{ref})$. At the moment of writing, an approximation of this relation as given by industry is

$$\tilde{g}(T, T_{ref}) = \left(\frac{T}{T_{ref}} \right)^{\frac{3}{2}} \exp \left(6400 \left(\frac{1}{T_{ref}} - \frac{1}{T} \right) \right). \quad (96)$$

So the function $g(T, T_{ref})$ relates the dark current of a given temperature to the dark current at the reference temperature: $S_{dc}(T, t_{exp}) = g(T, T_{ref}) S_{dc}(T_{ref}, t_{exp})$. The temperature stabilization of the detector is designed to be sufficiently stable to not cause significant changes in dark current during an orbit. The actual in-flight measurements and calibration measurements probably have different associated temperatures. If not, that is if $T = T_{ref}$, the function g equals 1.

A definite temperature relation will follow from actual on-ground calibration dark current measurements, performed at a range of temperatures. While the actual relation will probably resemble Equation 96 above, a more general description of g will be provided as a Chebyshev polynomial of the variable $x = T - T_{ref}$:

$$g(T, T_{ref}) = \sum_{j=0}^N c_j T_j(\tilde{x}) \quad (97)$$

Here the notation \tilde{x} means that the variable has been scaled between -1 and 1 , as usual. Further, $\tilde{x} = 0$ means that $T = T_{ref}$. See the Appendix for details on Chebyshev polynomials.

The choice of such a polynomial will also circumvent the implementation of the exponential function in the L01b Processor. Associated with g is its error function s_g^2 , similarly expressed with polynomial coefficients.

As mentioned before, the dark current can vary per detector pixel. The temperature is constant over the entire detector, and therefore over all detector pixels. We need the average dark current of the set of detector pixels that constitute an image pixel. This gives the correction step:

$$S_o[\mathbf{x}_{img}] = S_i[\mathbf{x}_{img}] - \left[\frac{\sum_{\mathbf{x}_{det} \in \mathbf{x}_{img}} f_{dc,image,T_{ref}}[\mathbf{x}_{det}]}{N_{\mathbf{x}_{det} \in \mathbf{x}_{img}}} \cdot (t_{exp} - t_{frametransfer}) + B + C + D \right] \cdot g(T, T_{ref}). \quad (98)$$

Note that the dark current correction is also performed for a background image, with its own associated temperature. After this correction, this background image can be considered a residual and be combined with other residuals, see Section 22.8.

22.7.3 Error propagation

We assume that the temperature difference $T - T_{\text{ref}}$ is measured exactly. Further, exposure time and storage time are assumed to contain no error. Then formal error propagation gives:

$$\begin{aligned} \sigma_0^2[\mathbf{x}_{\text{img}}] &= \sigma_i^2[\mathbf{x}_{\text{img}}] + g^2(T, T_{\text{ref}}) [s_a^2 + s_b^2 + s_c^2 + s_d^2] \\ &\quad + s_g^2(T, T_{\text{ref}}) \left[\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{dc,image},T_{\text{ref}}}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \cdot (t_{\text{exp}} - t_{\text{frametransfer}}) + B + C + D \right]^2, \text{ with:} \\ s_a^2 &= \overline{s_{\text{dc,image},T_{\text{ref}}}^2[\mathbf{x}_{\text{det}}]} (t_{\text{exp}} - t_{\text{frametransfer}})^2 \\ s_b^2 &= t_{\text{frametransfer}}^2 \left(\frac{1}{n_{\text{rows}}^2} \sum_{r'} s_{\text{dc,image}}^2[r', c_{\text{det}}] \right) \\ s_c^2 &= s_{\text{dc,storage},T_{\text{ref}}}^2 \cdot t_{\text{storage}}^2[r_{\text{img}}] \end{aligned} \quad (99)$$

Note that s_d^2 and the factor between brackets in s_b^2 are directly provided as CKD.

We use the definition of the mean unbinned variance described in Section 20.4.2:

$s_{\text{dc,image},T_{\text{ref}}}^2[\mathbf{x}_{\text{det}}] = \frac{1}{N} \sum s_{\text{dc,image},T_{\text{ref}}}^2[\mathbf{x}_{\text{det}}]$. Implicitly, we do not wish to assume that the individual dark currents in a bin are uncorrelated; otherwise the last term could be divided by the binning factor. This choice seems to contradict the definition of s_b^2 , where the factor n_{rows}^2 implies that, over all image rows combined, the correlation does not hold. We justify this as finding a balance between best- and worst case scenarios; moreover, the correlation between s_a^2 and s_b^2 is hard to assess.

22.8 Residual aggregate

For every instrument configuration, a dual, but dark, image of the illuminated image under consideration is provided. Such an image is taken as close in time as possible as the associated illuminated signal. Thus, all instrument settings are the same as for the corresponding illuminated images, except for the presence of the light source. Generally, for each illuminated instrument configuration, an entire measurement series of corresponding background images is taken. These background images can be combined; the combination is called an aggregate.

Note that the dark current correction (see Section 22.7) is also performed for each background image, with its own associated temperature. After this correction, this background image can be considered, and renamed, a residual. The combination of these residuals is called the residual aggregate. The construction of the residual aggregate is described in this section. This aggregate image can be used afterwards in the residual correction algorithm step (Section 22.9).

22.8.1 Used parameters and symbols

Parameter	Description	Units
k	enumerator for residual images	1
n_{res}	number of residual images	1
$S_{i,k}[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} for residual image k	e^-
$\sigma_{i,k}^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} for residual image k	e^{-2}
$S_{\text{res}}[\mathbf{x}_{\text{img}}]$	residual aggregate signal	e^-
$\sigma_{\text{res}}^2[\mathbf{x}_{\text{img}}]$	variance of residual aggregate signal	e^{-2}
$s_{\text{meas}}^2\{S_{\text{res}}[\mathbf{x}_{\text{img}}]\}$	measurement noise of residual aggregate signal	e^{-2}

22.8.2 Algorithm description

We suppose that n_{res} individual residual images are available. This number may be smaller than the original length of the background measurement series: low-quality images or images that deviate too much from the mean are discarded.

$$S_{\text{res}}[\mathbf{x}_{\text{img}}] = \frac{1}{n_{\text{res}}} \sum_{k=1}^{n_{\text{res}}} S_{i,k}[\mathbf{x}_{\text{img}}]. \quad (100)$$

22.8.3 Error propagation

The errors of the individual residuals will roughly be the same, due to the deterministic character of the L01b Processor. These errors are strongly correlated. Therefore, the combined error is not smaller than the individual errors. Instead, we define the combined error as the average of the individual errors. This is equivalent of assuming full correlation between the individual signals.

$$s_{\text{res}}^2[\mathbf{x}_{\text{img}}] = \frac{1}{n_{\text{res}}} \sum_{k=1}^{n_{\text{res}}} \sigma_{i,k}^2[\mathbf{x}_{\text{img}}] , \quad (101)$$

The measurement noises of the individual residuals, however, will be completely uncorrelated. The noise of the aggregate is therefore smaller than the noise of the individual residuals, according to Equation (38) in Section 20.3:

$$s_{\text{meas}}^2\{S_{\text{res}}[\mathbf{x}_{\text{img}}]\} = \frac{1}{n_{\text{res}}^2} \sum_{k=1}^{n_{\text{res}}} s_{\text{meas}}^2\{S_{i,k}[\mathbf{x}_{\text{img}}]\} . \quad (102)$$

22.8.4 Remark

If too few residual images are available, a fallback strategy is to use the residual CKD. This CKD has been constructed in the same way as the residual aggregate, and will be of high quality (concerning, for example, the signal-to-noise ratio) but is generally not collected as close in time as the illuminated images. The residual CKD contains per definition no noise; this has been incorporated in its error.

22.9 Residual correction

Apart from the actual illuminated signal, the signal recorded by the CCDs consists of a number of additional components. These components, all additive, need to be corrected for in the L01b Processor. We have already discussed the offset (Section 22.2); other components are dark current (Section 22.7) and smear (Section 22.10).

Measurements without illumination, the so-called background measurements, contain only a few of these additive components. At this stage in the L01b Processor, with the offset and the dark current already having been coped with, the background images (now renamed residual images) contain only unmodeled artefacts like electromagnetic compatibility (EMC) and, depending on its definition, pixel-to-pixel offset non-uniformity (PONU).

Note that the residual is defined per ICID and cannot be described in a more general way like the dark current (which can be modeled as a flux). A residual for zero exposure time cannot be defined: we would need a model for that. We can define PONU as a constant ICID-independent part of the residual. But this definition is merely academic. In any case, after the residual correction any electronic offset has per definition disappeared. In the residual correction algorithm, illuminated images are corrected with the aggregated residual signal of their associated background ICID. If the aggregated residual is not available, a fallback strategy is to use the residual CKD. This CKD has been constructed in the same way as the residual aggregate, and will be of high quality (concerning, for example, the signal-to-noise ratio) but is generally not collected as close in time as the illuminated images. The residual CKD contains per definition no noise; this has been incorporated in its error. After the residual subtraction, the error due to the offset should have disappeared. EMC, if it occurs, is a known unknown that is exactly the same for both illuminated and dark image. Hence, this term, no matter its contribution, cancels as well due to the residual correction.

This algorithm is related to Section 17.1 in the forward model part.

22.9.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
$S_{\text{res}}[\mathbf{x}_{\text{img}}]$	residual aggregate signal	e^-
$s_{\text{res}}^2[\mathbf{x}_{\text{img}}]$	variance (error) of residual aggregate signal	e^{-2}
$\sigma_{\mu,\text{res}}^2$	offset variance propagated to this algorithm step	e^{-2}
$s_{\text{dc}}^2[\mathbf{x}_{\text{img}}]$	variance increase due to dark current correction	e^{-2}

22.9.2 Algorithm description

The residual signal is subtracted from the current signal, in the binned sense:

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] - S_{\text{res}}[\mathbf{x}_{\text{img}}] . \quad (103)$$

22.9.3 Error propagation

An interesting aspect of the residual subtraction is that it may have, at least partly, an ameliorating effect on the error: The error on the offset subtraction cancels out if the offset does not depend on the temperature. Also, the dark current error will cancel. The offset error term has been introduced as s_{μ}^2 in Section 22.2 and has been propagated ever since. The total propagation effect is multiplicative; that is, the original offset variance s_{μ}^2 has been evolved towards

$$s_{\mu,\text{res}}^2 = \left(\frac{1}{n_{\text{bin}}^2} \cdot f_{\text{v}2\text{c}}^2 \cdot \frac{1}{G_{\text{sys}}^2} \right) s_{\mu}^2 . \quad (104)$$

If a significant dependence of the offset on the temperature exists, however, then Equation (104) is not valid and we have to set $s_{\mu,\text{res}}^2 = 0$. The variance of the binned residual signal can immediately be applied. Therefore the total error propagation is

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] - s_{\mu,\text{res}}^2 - s_{\text{dc}}^2[\mathbf{x}_{\text{img}}] + s_{\text{res}}^2[\mathbf{x}_{\text{img}}] . \quad (105)$$

A far better alternative than this bookkeeping is to skip the error propagation for the offset and dark current corrections (giving the smaller error $\sigma_{i,\text{red}}^2$ instead of σ_i^2) if beforehand it is known that the signal will be processed up to and including the residual correction algorithm. In that case, we simply have

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_{i,\text{red}}^2[\mathbf{x}_{\text{img}}] + s_{\text{res}}^2[\mathbf{x}_{\text{img}}] . \quad (106)$$

22.10 Smear

The purpose of the smear correction algorithm is to negate the effect of frame transfer smear, or smear for short in this context. Per definition, smear is the added contribution of the signal due to continued exposure during read-out. More specifically, each row continues to receive photons during its transfer through the CCD image section. The smear is therefore always positive and the correction should consist of a subtraction.

Since we have detailed knowledge of the row transfer process it is in principle possible to compute the exact amount of smear generated. However, in the reverse model we only have the measured (uncorrected) signal to start with. This signal contains less information than the original signal due to non-invertible operations like row binning and co-addition. The goal of the algorithm is to provide an inverted smear addition model that is as good as possible. This algorithm is related to Section 17.2 in the forward model part.

22.10.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
T	exposure time (excluding frame transfer time)	s
τ	row transfer time	s
n	number of detector rows: 1026	1
$n_{\text{unshielded}}$	number of unshielded detector rows	1
n_{shielded}	number of shielded detector rows (including two storage rows)	1
n_{usable}	number of unflagged (trusted), unskipped (readable), unshielded (illuminated) detector rows	1
m	number of binned (image) rows	1
f_r	signal rate in detector row r	$e^- \text{s}^{-1}$
g_r	signal rate in image row r	$e^- \text{s}^{-1}$
v_r	ROR signal in unbinned row r	e^-
w_r	ROR signal in binned row r	e^-
w_r'	ROR signal in binned row r after binning correction	e^-
a_r	factor between mean and start signal	1
b_r	factor between mean and end signal	1
$a_{r,i}$	factor between mean signal and end signal at co-add instance i	1
N_{coadd}	number of co-additions	1
M	smear	e^-
s_{smear}^2	Total increase of variance due to smear	e^-

22.10.2 Algorithm description: general

First we describe the creation of smear in the forward sense in more detail than in the forward model section. We start with the most general situation, in which all information is available. We then move to more realistic situations in which some assumptions have to be made. Since the smear is independent of columns, we only consider a single column on the CCD. The CCD has n unbinned rows; the first row is situated closest to the read-out register. *Note that we count here the amount of rows in the storage section: this is the number of rows that is actually transfered during a frame transfer and the frame transfer time is, per definition, $n\tau$. Although the amount of image section rows is 1024, we must not forget the extra two rows, and that they are in principle available for reading. Fortunately they can be considered shielded rows so we know their behaviour.* The development of the algorithm demands that we start with unbinned rows. Later on, we devote a section to the binned situation. Further, note that in this section T is the symbol for exposure time, not temperature.

Let f_r denote the signal rate on a pixel on row r due to illumination. This signal rate is, in general, not constant. We can define the signal rate more correctly by

$$f_r = \frac{1}{T} \int_{t_{\text{start}}}^{t_{\text{end}}} f(u) du, \quad (107)$$

where $t_{\text{end}} = t_{\text{start}} + T$. The variation of the scene, and hence of f_r , is important since the smear depends only on the signal rate $f_{r,t_{\text{start}}}$ and $f_{r,t_{\text{end}}}$. Consider a certain pixel on row r . Its cousin pixel 1 will enter the visual region from above at $t_{\text{start}} - n\tau$. The pixel r itself enters the CCD at $t_{\text{start}} - (n - r + 1)\tau$. During the first τ seconds, it briefly receives some electrons destined for the upper row; this amount of electrons is $\tau \cdot f_{n,t_{\text{start}} - (n-r+1)\tau}$. In the following τ seconds, some more (exactly: $\tau \cdot f_{n-1,t_{\text{start}} - (n-r+2)\tau}$) electrons are added. At this point we are, for practical reasons, forced to introduce our first assumption:

Assumption 1. The signal rate at pixel r between $t = t_{\text{start}} - n\tau$ and $t = t_{\text{start}}$ is assumed constant and denoted $f_{r,\text{start}}$.

We can justify this assumption by the fact that it is nearly impossible to observe changes in the scene on a

shorter timescale than $n\tau$ seconds. More important, the assumption is entirely harmless since in our forward smear model we will establish a relation between f_r and $f_{r,\text{start}}$. Any information we might obtain about the signal rate evolution between $t_{\text{start}} - n\tau$ and t_{start} can be incorporated in this relation.

This movement through the rows continues until the pixel reaches its designated position r , where it receives an additional $\tau \cdot f_{r,\text{start}}/2$ amount of electrons (the factor $1/2$ is evident when one considers that the center point of the pixel does not enter the pixel ‘box’ until the last $\tau/2$ seconds). Then, during the true exposure time, between t_{start} and t_{end} , the pixel receives its designated Tf_r electrons. After that, there are again $r - 1$ small time steps during which the pixel resides in the lower $r - 1$ positions, receiving, at each position k ($0 < k < r$), $\tau \cdot f_{k,\text{end}}$ electrons. Therefore we can express the relation between the illumination rate f and the ROR signal \mathbf{v} by the matrix equation

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = T \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix} + \tau \begin{pmatrix} \frac{1}{2} & 1 & 1 & \dots & 1 \\ 0 & \frac{1}{2} & 1 & \dots & 1 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & & \ddots & \frac{1}{2} & 1 \\ 0 & \dots & \dots & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} f_{1,\text{start}} \\ f_{2,\text{start}} \\ \vdots \\ f_{n,\text{start}} \end{pmatrix} + \tau \begin{pmatrix} \frac{1}{2} & 0 & 0 & \dots & 0 \\ 1 & \frac{1}{2} & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 1 & & \ddots & \frac{1}{2} & 0 \\ 1 & \dots & \dots & 1 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} f_{1,\text{end}} \\ f_{2,\text{end}} \\ \vdots \\ f_{n,\text{end}} \end{pmatrix}. \quad (108)$$

Our goal is to write the expression above as a single matrix-vector equation: $\mathbf{v} = \mathbf{A}\mathbf{f}$. The inverse of matrix \mathbf{A} can then be used in the reverse processor to acquire \mathbf{f} from \mathbf{v} . One way to achieve this goal is by expressing $f_{r,\text{start}}$ and $f_{r,\text{end}}$ into f_r . An easy solution is simply setting $f_{r,\text{start}} = f_{r,\text{end}} = f_r$. This choice, which we will call the pseudo-static variant from now on, will serve as a fall-back method. For scenes that vary strongly in the temporal dimension, this assumption can result in considerable errors in some pixels.

Although we do not have time-dependent information of the image itself, we can use the previous and following images. We can use the average signal rates of these frames, f_r^{prev} and f_r^{next} to obtain good guesses for $f_{r,\text{start}}$ and $f_{r,\text{end}}$; a simple linear interpolation (taking into account different exposure times) will do. Of course, at this stage we only have the read-out signal \mathbf{v} , not \mathbf{f} . Clearly, the problem is circular: the signal rate \mathbf{f} is not available before we solved the smear problem. But, at least, the read-outs \mathbf{v} for the frame considered and the previous and following images give a good approximation. For co-added scenes, the small-pixel columns typically provide temporal information. Later, we will elaborate on this aspect (see Section 22.10.4).

Regardless of the method we choose, we can write

$$f_{r,\text{start}} = \alpha_r f_r \quad (109a)$$

and

$$f_{r,\text{end}} = \beta_r f_r. \quad (109b)$$

The α_r and β_r will always be non-negative. Equation (108) can now be reduced. We first introduce $\varepsilon = \tau/T$ and then $a_i = \varepsilon\alpha_i$ and $b_i = \varepsilon\beta_i$. We get

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = T \begin{pmatrix} 1 + \frac{1}{2}(a_1 + b_1) & a_2 & a_3 & \dots & \dots & a_n \\ b_1 & 1 + \frac{1}{2}(a_2 + b_2) & a_3 & \dots & \dots & a_n \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \vdots \\ b_1 & & & \ddots & 1 + \frac{1}{2}(a_{n-1} + b_{n-1}) & a_n \\ b_1 & \dots & \dots & \dots & b_{n-1} & 1 + \frac{1}{2}(a_n + b_n) \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}. \quad (110)$$

The smear M is defined as the contribution outside the true exposure time interval, therefore:

$$\begin{aligned} M(\mathbf{v}) &= \mathbf{A}\mathbf{f} - T\mathbf{f} = (\mathbf{A} - T\mathbf{I})\mathbf{f} = \\ &= (\mathbf{A} - T\mathbf{I})\mathbf{A}^{-1}\mathbf{v} = (\mathbf{I} - \mathbf{A}^{-1}T)\mathbf{v}. \end{aligned} \quad (111)$$

Now we have expressed the smear in terms of the read-outs v_j . The f_j , which are not available before the smear correction, are no longer needed. Note further that, although M is a function of \mathbf{v} , it is the same for a pixels in the column: $M(v_i) = M(v_j) \forall i, j$; therefore we may also write $M(c_{\text{img}})$.

As an intermezzo, we note that in the pseudo-static variant (where the choice for α and β was simply $\alpha = \beta = 1$) \mathbf{A} reduces to

$$T \begin{pmatrix} 1 + \varepsilon & \varepsilon & \dots & \dots & \varepsilon \\ \varepsilon & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \varepsilon \\ \varepsilon & \dots & \dots & \varepsilon & 1 + \varepsilon \end{pmatrix}. \quad (112)$$

As remarked above, this choice can produce considerable errors. An advantage is that the matrix is easy to invert. Having established this exact result, the smear correction problem boils down to the following questions:

1. How accurately can the coefficients a_i and b_i be chosen?
2. In what way will row binning influence the result?
3. In what way will row skipping influence the result?
4. How can we incorporate co-adding using this result?
5. Is the inverse of the matrix \mathbf{A} easily computed?

These questions are interrelated. For example, more binning and skipping decreases the accuracy of the coefficients a_i and b_i . Some choices of the coefficients permit a simpler matrix structure regarding inversion.

22.10.3 Algorithm description: binning and skipping

We consider the effect of binning and skipping, without taking the binning factor division into account. Suppose there are m binned rows. w_j is the binned signal in the read-out register, and g_j the illumination rate. The w_j and g_j have the same binning factor n_j . We need some more administration in the form of a binning table. Define q_j^{start} and q_j^{end} as a mapping from image row j , towards the corresponding rows on the CCD. It always holds that $q_j^{\text{start}} + n_j - 1 = q_j^{\text{end}}$. Further, $q_j^{\text{start}} = q_{j-1}^{\text{end}} + 1$. Clearly

$$g_j = \sum_{i=0}^{n_j} f_{i+q_j^{\text{start}}}, \quad w_j = \sum_{i=0}^{n_j} v_{i+q_j^{\text{start}}}. \quad (113)$$

Our strategy regarding skipped rows is to assume, for as long as possible, as if no rows are skipped at all. This makes sense since the rows considered are binned with their own binning factors like normal rows. The only difference is that, in the end, the information is discarded.

The binning matrix \mathbf{B} has dimensions $m \times n$ and has a simple shape: row j contains zeroes except for the entries between column q_j^{start} and column q_j^{end} , which are filled with n_j ones. The matrix \mathbf{B} is not invertible, so the construction $\mathbf{w} = \mathbf{Bv} = \mathbf{BAf} = \mathbf{BAB}^{-1}\mathbf{g}$ will not work. Instead, we explicitly try to write down $\mathbf{w} = \mathbf{BAf}$. Since we only have binned information available, we cannot determine the exact values of a_i and b_i . We are therefore forced to invoke the following assumption:

Assumption 2. The a_i and b_i in rows belonging to the same bin j are all equal.

Define $a_j^b = a_{q_j^{\text{start}}} = a_{q_j^{\text{start}}+1} = \dots = a_{q_j^{\text{end}}}$ and a similar definition for b_j^b . Now $\mathbf{w} = \mathbf{BAf}$ where $\mathbf{w} = (w_1 \dots w_m)^T$ and \mathbf{BA} is the $m \times n$ matrix

$$T \begin{pmatrix} 1 + \frac{1}{2}a_1^b + (n_1 - \frac{1}{2})b_1^b & \dots & 1 + (n_1 - \frac{1}{2})a_1^b + \frac{1}{2}b_1^b & n_1a_2^b & \dots & n_1a_m^b \\ n_2b_1^b & \dots & n_2b_1^b & 1 + \frac{1}{2}a_2^b + (n_2 - \frac{1}{2})b_2^b & \dots & n_2a_m^b \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ n_{m-1}b_1^b & & \ddots & \ddots & \ddots & n_{m-1}a_m^b \\ n_mb_1^b & \dots & \dots & \dots & \dots & 1 + (n_m - \frac{1}{2})a_m^b + \frac{1}{2}b_m^b \end{pmatrix}. \quad (114)$$

For a certain entry w_j we get

$$w_j = \sum_{i=1}^{j-1} \sum_{k=q_i^{\text{start}}}^{q_i^{\text{end}}} n_j b_i^b f_k + \sum_{i=j+1}^m \sum_{k=q_i^{\text{start}}}^{q_i^{\text{end}}} n_j b_i^b f_k + \sum_{k=q_j^{\text{start}}}^{q_j^{\text{end}}} [1 + (\tilde{k} - \frac{1}{2})a_j^b + (n_j - \tilde{k} - \frac{1}{2})b_j^b] f_k, \quad (115)$$

with, in the last term, $\tilde{k} = k - q_j^{\text{start}} + 1$. The first term of this expression reduces to

$$n_j \sum_{i=1}^{j-1} b_i^b \sum_{k=q_i^{\text{start}}}^{q_i^{\text{end}}} f_k = n_j \sum_{i=1}^{j-1} b_i^b g_i \quad (116)$$

and a similar expression holds for the second term. To reduce the third term, we need another assumption:

Assumption 3. The convolution $\sum_{k=q_j^{\text{start}}}^{q_j^{\text{end}}} [1 + (\tilde{k} - \frac{1}{2})a_j^b + (n_j - \tilde{k} - \frac{1}{2})b_j^b] f_k$ may be simplified to

$$[1 + \frac{1}{2}n_j(a_j^b + b_j^b)] \sum_{k=q_j^{\text{start}}}^{q_j^{\text{end}}} f_k . \quad (117)$$

In effect, the mean of the term between square brackets is taken. This assumption introduces an error if the f_k are not all equal. We now have reached the matrix equation

$$\mathbf{w} = \mathbf{C}\mathbf{g} , \quad (118)$$

where \mathbf{C} is an $m \times m$ matrix:

$$T \begin{pmatrix} 1 + \frac{1}{2}n_1(a_1^b + b_1^b) & n_1a_2^b & n_1a_3^b & \dots & \dots & n_1a_m^b \\ n_2b_1^b & 1 + \frac{1}{2}n_2(a_2^b + b_2^b) & n_2a_3^b & \dots & \dots & n_2a_m^b \\ \vdots & \ddots & \ddots & \ddots & \dots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ n_{m-1}b_1^b & & \ddots & 1 + \frac{1}{2}n_{m-1}(a_{m-1}^b + b_{m-1}^b) & n_{m-1}a_m^b \\ n_mb_1^b & \dots & \dots & n_mb_{m-1}^b & 1 + \frac{1}{2}n_m(a_m^b + b_m^b) \end{pmatrix} . \quad (119)$$

Note the similarities between the unbinned equation (110) and this binned equation (118). In particular, the two equations become the same if all n_j are equal to 1. The smear is, as before, defined as the contribution outside the true exposure time interval, therefore:

$$M(\mathbf{w}) = \mathbf{C}\mathbf{g} - T\mathbf{g} = (\mathbf{C} - T\mathbf{I})\mathbf{g} = (\mathbf{C} - T\mathbf{I})\mathbf{C}^{-1}\mathbf{w} = (\mathbf{I} - \mathbf{C}^{-1}T)\mathbf{w} . \quad (120)$$

At this point we finally have to take the possibility of skipped rows into account. Suppose the binned row r is skipped. In Equation (118), this means the following:

- The read-out value w_r is actually not read out, by definition. However, it is needed in the right-hand side of Equation (120). Therefore we need to interpolate the w_r from the neighboring binned w_{r-k}, \dots, w_{r+k} pixels in the same column.
- The binned illumination g_r is not needed since it will not be used in Equation (120).
- In matrix \mathbf{C} , the cross consisting of row r and column r can be highlighted. The matrix row will not be used, but the matrix column, including the coefficients a_r and b_r is needed to compute the unskipped entries of \mathbf{w} . Eventually, however, we need \mathbf{C}^{-1} . That means we have guess the coefficients a_r and b_r (in the pseudo-static approach, they are of course equal to 1). The coefficients can be interpolated from neighboring columns. If the skipped row has special characteristics (if the row is in a straylight area or is not illuminated) care must be taken; a fallback strategy is to choose $a_r = b_r = 1$.

Concluding, the equations stay the same, and the unknowns a_r, b_r and w_r are estimated by interpolation.

The interpolation of the skipped pixel w_r can be done in several ways:

- Direct linear interpolation from the previous and next binned row. At top and bottom, extrapolation has to be used. Further, if the skipped row is different in terms of illumination/shielding from neighboring rows, the interpolation will not yield good results.

- Extrapolation from the total unskipped column sum. That means that the column sum of all the available binned pixels is multiplied with a factor $n_{\text{unshielded}}/n_{\text{usable}}$ where the denominator contains the number of unskipped pixels expressed in the amount of the associated detector pixels. A disadvantage is that it is less accurate since the extrapolation is global, not local. Note that in both the numerator and the denominator we only count the pixels that are expected to have a properly illuminated signal; hence the exclusion of shielded pixels.
- Extrapolation from a total unskipped partial column sum. A partial column is for example the union of all 'illuminated pixels'. Here each skipped pixel can belong to a group with the same characteristics (shielded, non-illuminated, illuminated). The same disadvantage as the second method holds.

Since we expect that skipped rows will be extremely rare, the baseline is the second (easiest) method.

22.10.4 Algorithm description: co-addition

When we take co-addition into account, some things change, some things stay the same. Note that Equation (108) refers to a single frame in a co-added series. We introduce some notation. Forgetting binning for the moment, we still assume we have n detector rows. Suppose the image is a sum of N_{coadd} frames. The total amount of time that the image will be illuminated is $T_{\text{illum,tot}} = N_{\text{coadd}}(T + n\tau)$ s. Using Assumption 1, we define the times where smear is added as t_0 (this is the t_{start} described above), $t_1, t_2, \dots, t_{N_{\text{coadd}}}$. As explained before, these times are in reality time intervals of length $n\tau$. Further, we define the mean signal rate for frame i as

$$f_r^i = \frac{1}{T} \int_{t_{\text{start};i}}^{t_{\text{end};i}} f(u) du, \quad (121)$$

where $t_{\text{end};i} = t_{\text{start};i} + T$. For a pixel in row r we get:

$$\begin{aligned} v_r &= \tau \sum_{j=r+1}^n f_{j,t_0} + T f_r^1 + \tau \sum_{j=1}^{r-1} f_{j,t_1} + \frac{1}{2} \tau (f_{r,t_0} + f_{r,t_1}) \\ &+ \tau \sum_{j=r+1}^n f_{j,t_1} + T f_r^2 + \tau \sum_{j=1}^{r-1} f_{j,t_2} + \frac{1}{2} \tau (f_{r,t_1} + f_{r,t_2}) \\ &+ \dots \\ &+ \tau \sum_{j=r+1}^n f_{j,t_{N_{\text{coadd}}-1}} + T f_r^{N_{\text{coadd}}} + \tau \sum_{j=1}^{r-1} f_{j,t_{N_{\text{coadd}}}} + \frac{1}{2} \tau (f_{r,t_{N_{\text{coadd}}-1}} + f_{r,t_{N_{\text{coadd}}}}). \end{aligned} \quad (122)$$

This can be simplified to:

$$\begin{aligned} v_r &= \tau \sum_{i=r+1}^n f_{i,t_0} + T \sum_{i=1}^{N_{\text{coadd}}} f_r^i + \tau \sum_{i=1}^{N_{\text{coadd}}-1} \left(\sum_{j=1}^n f_{j,t_i} \right) \\ &+ \tau \sum_{j=1}^{r-1} f_{j,t_{N_{\text{coadd}}}} + \frac{1}{2} \tau (f_{r,t_0} + f_{r,t_{N_{\text{coadd}}}}). \end{aligned} \quad (123)$$

This expression should be incorporated into a matrix equation similar to Equation 110. That means we define the average signal rate f_r as

$$f_r = \frac{1}{N_{\text{coadd}}} \sum_{i=1}^{N_{\text{coadd}}} f_r^i \approx \frac{1}{T_{\text{illum,tot}}} \int_{t_0}^{t_{N_{\text{coadd}}}} f(u) du. \quad (124)$$

Further, we have to establish relations between f_r and all $N_{\text{coadd}} + 1$ signal rates during the frame transfers. So, instead of just choosing a_i and b_i following Equations (109a) and (109b) in the case without co-additions, we define

$$f_{r,t_i} = \alpha_{r,i} f_r, \quad 1 \leq r \leq n; \quad 0 \leq i \leq N_{\text{coadd}}. \quad (125)$$

The resulting matrix has a similar structure as in Equation (110), using again $a_{r,i} = (\tau/T) \alpha_{r,i}$, with on the diagonal:

$$A_{r,r} = T(N_{\text{coadd}} + \frac{1}{2} a_{r,0} + a_{r,1} + \dots + a_{r,N_{\text{coadd}}-1} + \frac{1}{2} a_{r,N_{\text{coadd}}}), \quad (126)$$

below the diagonal:

$$A_{r,q} = T \sum_{i=1}^{N_{\text{coadd}}} a_{q,i} \quad 1 \leq q < r \leq n, \quad (127)$$

and above the diagonal:

$$A_{r,q} = T \sum_{i=0}^{N_{\text{coadd}}-1} a_{q,i} \quad 1 \leq r < q \leq n. \quad (128)$$

Here we see again that the entries in a column q are independent of the row number r . When we finally move to the binned situation, invoking Assumptions 2 and 3 for each individual frame transfer, we obtain again the row dependency in terms of the binning factor similar as in Equation (118). We return to the discussion on how to obtain the factors $\alpha_{j,i}$. The small-pixel column provides a possibility to obtain some temporal information. Fortunately, the correlation between the small-pixel column and the other columns in the same image is rather high.

Therefore, $\alpha_{r,i}$, $0 \leq i \leq N_{\text{coadd}}$, $1 \leq r \leq n$ can be chosen as the average of the values in the small-pixel columns for co-additions i and $i - 1$. For $\alpha_{r,0}$, the last small-pixel column of the previous image together with the small-pixel column of frame 0 should be used; for $\alpha_{r,N_{\text{coadd}}}$, the first small-pixel column of the next image together with the small-pixel column of frame N_{coadd} . Moreover, we have the *complete* previous and next images; these help in making good estimates of time gradients and prevent us to be completely dependent on the small-pixel column estimates.

In the pseudo-static approach the matrix \mathbf{A} can be simplified: It reduces, after dividing by N_{coadd} , to the matrix in Equation (112) in the unbinned case and to a similarly simplified version of \mathbf{C} in Equation (118) in the binned case.

22.10.5 Algorithm description: computing the inverse of the matrix

We can explicitly compute the inverse with the Gauss algorithm. This does not involve many computations: after swapping the bottom and top rows, one sweep will create an upper triangular matrix except for the bottom row. After elimination of that bottom row, inverse substitution immediately gives the inverse. This inverse can be computed for each image column (if we choose different factors $\alpha_{j,i}$ for each image column) or for all image columns simultaneously (if we only make use of the small-pixel columns in our choices of $\alpha_{j,i}$).

An alternative is to use Gauss-Seidel iterations. There are two approaches. Either we try to find a solution for each (of the more than 1000) column vector \mathbf{v} or we construct all m columns of the matrix using the columns of the identity matrix of size m . Our first iteration guess in the latter case would be the inverse matrix in the pseudo-static approach (see immediately below). Whatever choice will be made, restrictions for the computational time have to be taken into account.

In the pseudo-static approach the matrix inverse can be written down directly (and, therefore, fast):

$$\mathbf{C}^{-1} = \frac{1}{T(1+n\epsilon)} \begin{pmatrix} 1 + \epsilon(n - n_1) & -n_1\epsilon & -n_1\epsilon & \dots & \dots & -n_1\epsilon \\ -n_2\epsilon & 1 + \epsilon(n - n_2) & -n_2\epsilon & \dots & \dots & -n_2\epsilon \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ -n_{m-1}\epsilon & & & \ddots & 1 + \epsilon(n - n_{m-1}) & -n_{m-1}\epsilon \\ -n_m\epsilon & \dots & \dots & \dots & -n_m\epsilon & 1 + \epsilon(n - n_m) \end{pmatrix}. \quad (129)$$

Applying the formula for smear (Equation (120)) for a signal in binned row r immediately gives

$$M(w_r) = (\mathbf{I} - \mathbf{C}^{-1}T) \mathbf{w}_r = \frac{1}{1+n\epsilon} \sum_{j=1}^m n_r \epsilon w_j = n_r \frac{\tau}{T+n\tau} \sum_{j=1}^m w_j. \quad (130)$$

However, the smear correction takes place after the binning correction step. Define the measured signal after binning correction $w'_r = w_r/n_r$. In vector form, $\mathbf{w}' = \mathbf{N}^{-1} \mathbf{w}$, where $\mathbf{N} = \text{diag}(n_1, n_2, \dots, n_m)$. Then

$$M(\mathbf{w}') = M(\mathbf{N}^{-1} \mathbf{w}) = (\mathbf{I} - \mathbf{C}^{-1}T) \mathbf{N}^{-1} \mathbf{w} = \mathbf{N}^{-1} M(\mathbf{w}) \quad (131)$$

and for a signal after binning division in binned row r this gives

$$M(w'_r) = \frac{1}{n_r} M(w_r) = \frac{\tau}{T+n\tau} \sum_{j=1}^m n_j w'_j, \quad (132)$$

where w'_r is of course the measured signal $S_i[\mathbf{x}_{\text{img}}]$.

We claim that the smear correction works as a simple multiplicative operation on the column average and (by extension) image average: We have

$$S_o[r_{\text{det}}] = S_i[r_{\text{det}}] - \frac{\tau}{T + n\tau} \bar{S}_i \quad (133)$$

where the \bar{S}_i denotes the signal average over all rows in a column. Then for the column average we have

$$\bar{S}_o = \frac{1}{n} \sum_{r_{\text{det}}=1}^n S_o[r_{\text{det}}] \quad (134)$$

$$= \frac{1}{n} \sum_{r_{\text{det}}=1}^n \left(S_i[r_{\text{det}}] - \frac{\tau}{T + n\tau} \bar{S}_i \right) \quad (135)$$

$$= \bar{S}_i - \frac{\tau}{T + n\tau} \bar{S}_i = \left(1 - \frac{\tau}{T + n\tau} \right) \bar{S}_i. \quad (136)$$

22.10.6 Practical aspects

When computing the column sum, we encounter the practical problem that the we assumed that each pixel signal can be measured. Because the image section is two rows smaller than the storage section, this may not be the case. Also, pixels may be unavailable (skipped) /untrustworthy (flagged). We cope with this problem in two steps. First, we know beforehand the number and location of shielded pixels. These pixels receive no light flux and they will therefore only contain the smear signal. The two storage section pixels can also be considered as shielded. These pixels can be split from the summation and moved to the left-hand side of the equation:

$$M(w'_r) = M(c_{\text{img}}) = \frac{\tau}{T + n\tau} \sum_{j=1}^m n_j S_i[j] = \frac{\tau}{T + n\tau} \left(\sum_{\text{unshielded, binned}} n_j S_i[j] + \sum_{\text{shielded, binned}} n_j S_i[j] \right) \quad (137)$$

$$= \frac{\tau}{T + n\tau} \sum_{\text{unshielded, binned}} n_j S_i[j] + \frac{\tau}{T + n\tau} n_{\text{shielded}} M(c_{\text{img}}) \quad (138)$$

$$\implies \frac{T + n\tau - n_{\text{shielded}} \tau}{T + n\tau} M(c_{\text{img}}) = \frac{\tau}{T + n\tau} \sum_{\text{unshielded, binned}} n_j S_i[j] \quad (139)$$

$$\implies M(c_{\text{img}}) = \frac{\tau}{T + \tau(n - n_{\text{shielded}})} \sum_{\text{unshielded, binned}} n_j S_i[j]. \quad (140)$$

Now we have to decide how to handle flagged pixels. The baseline philosophy is that flagged pixels are unreliable and should not be used on right-hand side of an equation. Therefore we treat a flagged pixel as 'skipped': we extend the unreliability to the policy that we do not possess any information. Baseline is again that we extrapolate from the total unskipped column sum. That means that the column sum of all the available non-flagged binned pixels is multiplied with a factor $f_{\text{column-scaling}} = n_{\text{unshielded}}/n_{\text{usable}}$ where the denominator contains the number of unflagged/unskipped pixels expressed in the amount of the associated detector pixels. Note that in both the numerator and the denominator we have already excluded the shielded pixels. Therefore, we write

$$M(c_{\text{img}}) \approx \frac{\tau}{T + (n - n_{\text{shielded}}) \tau} f_{\text{column-scaling}} \sum_{\text{usable binned pixels}} n_j S_i[q, c]. \quad (141)$$

We stress that the summation index q involves only the image rows in the unshielded region that are available to read and do not contain any flags.

22.10.7 On two approaches

We will first assess the following trade-off: We can use the pseudo-static approach (which does not need any information beside the image itself, and provides an easy inverse matrix) but introduces an error due to the time dependency. On the other hand, we can use the potentially exact approach involving the three assumptions and the estimates that have to be made, while the matrix inversion is less simple.

We start with some estimates for the co-added, unbinned case. The smear computed according to the pseudo-static approach in a row r , as a function of the signal rate, is

$$M_{\text{psa}}(r) = \tau \sum_{j=1}^n f_j = \tau n \bar{\mathbf{f}} \quad (142)$$

where $\bar{\mathbf{f}}$ is the flow rate averaged over all rows of the averaged (over the entire illumination period) signal rate \mathbf{f} (Equation (124)). We again define the average signal rate in terms of the flow rates of individual frames (see Equation (121)) as

$$f_r = \frac{1}{N_{\text{coadd}}} \sum_{i=1}^{N_{\text{coadd}}} f_r^i \approx \frac{1}{2N_{\text{coadd}}} \sum_{i=1}^{N_{\text{coadd}}-1} (f_{r,t_i} + f_{r,t_{i+1}}) = \dots, \quad (143)$$

while we note that the equality holds for piecewise linear behavior of the individual flow rates. The approximation becomes worse for lower numbers of co-additions. We continue:

$$\dots = \frac{1}{N_{\text{coadd}}} \left[\frac{1}{2}(f_{r,t_0} + f_{r,t_{N_{\text{coadd}}}}) + \sum_{i=1}^{N_{\text{coadd}}-1} f_{r,t_i} \right] = f_r \frac{1}{N_{\text{coadd}}} \left[\frac{1}{2}(\alpha_{r,0} + \alpha_{r,N_{\text{coadd}}}) + \sum_{i=1}^{N_{\text{coadd}}-1} \alpha_{r,i} \right]. \quad (144)$$

This gives a useful property of the $\alpha_{r,i}$. We use this to expand Equations (126) through (128):

$$A_{r,r} = T(N_{\text{coadd}} + \frac{\tau}{T}N_{\text{coadd}}) = (T + \tau)N_{\text{coadd}}, \quad (145)$$

$$\begin{aligned} A_{r,q,LD} &= T\left(\sum_{i=1}^{N_{\text{coadd}}-1} \alpha_{q,i} + \alpha_{q,N_{\text{coadd}}}\right) = T\left(\left[\sum_{i=1}^{N_{\text{coadd}}-1} \alpha_{q,i} + \frac{1}{2}(\alpha_{q,0} + \alpha_{q,N_{\text{coadd}}})\right] + \frac{1}{2}(\alpha_{q,N_{\text{coadd}}} - \alpha_{q,0})\right) \\ &= \tau([N_{\text{coadd}}] + \frac{1}{2}(\alpha_{q,N_{\text{coadd}}} - \alpha_{q,0})), \end{aligned} \quad (146)$$

$$A_{r,q,UD} = \tau([N_{\text{coadd}}] + \frac{1}{2}(\alpha_{q,0} - \alpha_{q,N_{\text{coadd}}})) , \quad (147)$$

The smear expressed in flow rates is therefore

$$\begin{aligned} N_{\text{coadd}}M(r) &= \sum_{q=1}^n A_{r,q}f_q = \tau N_{\text{coadd}} \sum_{q=1}^n f_q + \frac{1}{2}\tau \left[\sum_{q=1}^{r-1} (\alpha_{q,N_{\text{coadd}}} - \alpha_{q,0})f_q + \sum_{q=r+1}^n (\alpha_{q,0} - \alpha_{q,N_{\text{coadd}}})f_q \right] = \\ &= \tau N_{\text{coadd}} n \bar{\mathbf{f}} + \frac{1}{2}\tau \left[\sum_{q=1}^{r-1} (f_{q,t_{N_{\text{coadd}}}} - f_{q,t_0}) + \sum_{q=r+1}^n (f_{q,t_0} - f_{q,t_{N_{\text{coadd}}}}) \right]. \end{aligned} \quad (148)$$

After division by the co-addition factor, we recognize in the first term the smear $M_{\text{psa}}(r)$.

We pause here for a moment: in this derivation we see that we are able to upgrade the pseudo-static approach to the nonstatic approach once we have the scaling factors for (only) the first and last co-addition. In this way we do not need the difficult matrix inversion described above. Keeping this in mind, we continue:

We want to quantify the maximum error that will be made in the pseudo-static approach (Equation (142)). For row r , we can achieve a maximum error by maximizing $f_{q,t_0} - f_{q,t_{N_{\text{coadd}}}}$ for $q > r$ and, simultaneously, maximizing $f_{q,t_{N_{\text{coadd}}}} - f_{q,t_0}$ for $q < r$. Consider the maximum intensity factor of a changing scene to be K , i.e.

$$\frac{1}{K} \leq \frac{f_{p,t_i}}{f_{p,t_j}} \leq K, \quad \text{for all rows } p \text{ and all times } t_i, t_j. \quad (149)$$

In words, the maximum contrast in a column is the maximum of all temporal pixel contrasts in a column.

We now define a low flow rate f_L and a high flow rate $f_H = K f_L$. Further, an error in the smear is most critical if it adds to a low-signal pixel. We therefore find for the maximum relative error in the smear

$$\frac{M_{\text{max}} - M_{\text{psa}}}{f_L(T + n\tau)} = \frac{1}{2}\tau(K - 1)n \frac{1}{(T + n\tau)N_{\text{coadd}}}. \quad (150)$$

An example of such a scene is a high signal for negative cross-track angles in the first half of a co-addition period combined with a high signal for positive cross-track angles in the second half of the co-addition period: a 2 x 2 checkerboard pattern.

We see that the maximum error is independent of the number of co-additions given the integration time $N_{\text{coadd}}(T + n\tau)$. For the choices $K = 15$, $\tau = 0.75 \times 10^{-6}$ s, $n = 1026$ and $(T + n\tau)N_{\text{coadd}} = 1.08$ s, the relative error does not exceed 0.5%.

22.10.8 Error propagation

The error increase of this algorithm step will stem purely from the reconstruction process, since there are no CKD parameters involved. We will address the possible sources of error, without going into much detail yet:

- Determination of coefficients a_r, b_r (or $a_{j,i}$ in the co-added case). Computed factors far from one are suspicious and can introduce large errors. Small-pixel columns contain more noise than the signal and applying them to other columns introduces new errors. The fall-back approach is to choose $a_r = b_r = 1$ for all r .
- Concerning Assumption 1. This effect is expected to be incorporated in the choice of the coefficients.
- Concerning Assumptions 2 and 3. The error will be a function of the gradients of the detector pixels belonging to the same bin. These assumptions were necessary to derive the matrix \mathbf{C} . Errors are expected to be smaller than those of the derivation of the factors themselves.
- Concerning skipped rows. Many neighboring skipped rows covering an unexpected image gradient (for example, rows in a straylight area) can be the source of a significant error. The baseline of linear interpolation from neighboring visible rows will limit this error considerably.
- The computation of the matrix inverse. The inverse is either exact or will be acquired by some iteration algorithm, while the stop criterion can be set as strictly as needed. The variances will not change in a significant way.
- Concerning number of co-additions and exposure times. The amount of smear is roughly related to the ratio of row transfer time and exposure time. If we keep the integration time constant, the effects of lower exposure times are exactly balanced by the higher number of co-additions.
- The measurement itself is used for the correction. In particular, the transfer from v to f is influenced by shotnoise and read-out noise. This has to be taken into account.

An assessment of some scenarios, including the ‘hole in the clouds’ scenario, can help providing estimates for the remaining error after using the smear correction algorithm. The error term is expected to be small for stationary images without skipped rows, while the pseudo-static approach will perform worse for scenarios that vary during the integration time.

Because the pseudo-static approach will be the baseline, we formulate the error in more detail. From the list above, the coefficients and the matrix inverse are known and give no error. The three assumptions are no longer needed. That leaves, besides the formal error propagation (directly following from our model equation), three error sources: noise, time-varying scenes and (possibly) skipped rows. Note that, even if row skipping has not been planned in a configuration, a pixel that has been flagged as transient effectively has to be treated as a skipped pixel since the value of its signal is unknown.

Formal error propagation from the smear correction According to equation Equation (132), the signal in a row r changes due to a multiplication and an additive term based on all other signals in the column c :

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] - M(S_i[\mathbf{x}_{\text{img}}]) = S_i[\mathbf{x}_{\text{img}}] - \frac{\tau}{T + n\tau} \sum_{q=1}^m n_q S_i[q, c] \quad (151)$$

$$= \left(1 - \frac{\tau n_r}{T + n\tau}\right) S_i[\mathbf{x}_{\text{img}}] - \frac{\tau}{T + n\tau} \sum_{q \neq r} n_q S_i[q, c] \quad (152)$$

For the error propagation, the best-case scenario is a full correlation of all signals in the entire column: it results in an error multiplier smaller than one. We assume here, however, that the signals in the column are uncorrelated. This assumption is still rather conservative: a negative correlation between signal $S_i[\mathbf{x}_{\text{img}}]$ and the other signals in the column is unlikely, given our knowledge of the instrument. We therefore get for the *modeled* error propagation

$$s_{\text{model}}^2[\mathbf{x}_{\text{img}}] = \left(1 - \frac{\tau n_r}{T + n\tau}\right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + \left(\frac{\tau}{T + n\tau}\right)^2 \sum_{q \neq r} n_q^2 \sigma_i^2[q, c]. \quad (153)$$

As above, we might approximate the summation as

$$\sum_{q \neq r} n_q^2 \sigma_i^2[q, c] \approx f_{\text{column-scaling}} \sum_{q \neq r; \text{ usable}} n_q^2 \sigma_i^2[q, c]. \quad (154)$$

Noise We start with Equation (132). The propagated measurement noise for each binned pixel $s_{\text{meas}}^2[\mathbf{x}_{\text{img}}]$ is available; it has been corrected for the binning factor. This gives, similar as for the error:

$$s_{\text{noise}}^2[\mathbf{x}_{\text{img}}] = \left(\frac{\tau}{T+n\tau}\right)^2 \sum_{q \neq r} n_q^2 s_{\text{meas}}^2[q, c]. \quad (155)$$

where again

$$\sum_{q \neq r} n_q^2 s_{\text{meas}}^2[q, c] \approx f_{\text{column-scaling}} \sum_{q \neq r; \text{ usable}} n_q^2 s_{\text{meas}}^2[q, c]. \quad (156)$$

This component of the error will be optional as its magnitude seems negligible. Note that the noise of the pixel signal itself does not change since this is an additive algorithm.

Time-varying scenes We use Equation (148). This is a better approximation than the worst-case scenario described in Equation (150).

The small-pixel column can be used to estimate the scaling factors $\alpha_{q,0}$ and $\alpha_{q,N_{\text{coadd}}}$. The flux f_q can be approximated with $S[q, c_{\text{img}}]/(T+n\tau)$.

So we set, using the notation c_{spc} for the image column that is associated with the small pixel column: $\alpha_{q,t_0} = w'_{\text{spc}}[q][1]/w'[q, c_{\text{spc}}]$ and $\alpha_{q,t_{N_{\text{coadd}}}} = w'_{\text{spc}}[q][N_{\text{coadd}}]/w'[q, c_{\text{spc}}]$ for a binned pixel q . The two summations in Equation (148) must be performed in the binned sense, therefore

$$s_{\text{nonstatic}}^2[\mathbf{x}_{\text{img}}] = \left[\frac{1}{2} \frac{\tau}{(T+n\tau)N_{\text{coadd}}} \left(\sum_{q=1}^{r_{\text{img}}-1} n_q S[q, c_{\text{img}}] (\alpha_{q,t_{N_{\text{coadd}}}} - \alpha_{q,t_0}) + \sum_{q=r_{\text{img}}+1}^m n_q S[q, c_{\text{img}}] (\alpha_{q,t_0} - \alpha_{q,t_{N_{\text{coadd}}}}) \right) \right]^2 \quad (157)$$

Note that the summation should ignore flagged pixels; potential effects can be expected to cancel.

From these formula we see that the error for one co-addition is estimated to be zero, which of course need not to be the case. Because of the assumption of piecewise linear approximation, only the small pixel data for the first and last co-addition have to be used. A better approximation would be achieved if we also use the small pixel columns from the previous and next image. Further, if the scene is monotonous in the across-track direction, then the largest errors will occur at both low and high row numbers. Finally, the sum between brackets is again largest for a 2x2 checkerboard pattern (temporally increasing signals in low-numbered rows combined with temporally decreasing signals in high-numbered rows or vice versa).

Skipped rows In a skipped row r , we use an estimate for the unknown w_r : The signal is interpolated from neighboring signals. The worst case scenario is that the skipped row does not receive any light, such that the order or magnitude of the error is the same as the neighboring signals (the even worse alternative, that the skipped signal is more than a factor of two stronger than its neighbors, can be dispensed with as unrealistic). Equation (132) can be split in two:

$$M(w'_r) = \frac{\tau}{T+n\tau} \left[\sum_{j \text{ not skipped}} n_j w'_j + \sum_{j \text{ skipped}} n_j w'_j \right]. \quad (159)$$

Therefore, we can estimate the skip error as

$$\sigma_{\text{skip}}^2[c_{\text{img}}] = \left[\frac{1}{2} \frac{\tau}{T+n\tau} \sum_{j \text{ skipped}} n_j (S[j-1] + S[j+1]) \right]^2 \quad (160)$$

On reflection, the policy of this error component may be too harsh. We therefore decide to skip this term and instead decrease the quality number of the pixels in the column.

We set

$$Q[\mathbf{x}_{\text{img}}] = \max \left(0, Q[\mathbf{x}_{\text{img}}] - \alpha \left(1 - \frac{1}{f_{\text{column-scaling}}} \right) \right) \quad (161)$$

The factor α is an algorithm parameter between 0 and 1 that can ameliorate the negative effect on the quality number.

For completeness, we give the formal propagation:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = s_{\text{model}}^2[\mathbf{x}_{\text{img}}] + s_{\text{nonstatic}}^2[\mathbf{x}_{\text{img}}] + \mathbf{I}_{\text{include-noise-term}} s_{\text{noise}}^2[\mathbf{x}_{\text{img}}] \quad (162)$$

22.10.9 Remarks and alternatives

Instead of trying to determine factors α_i and β_i for the relation between f_i and $f_{i,start}$ and $f_{i,end}$, we can establish a regression line for all rows at once between f_i on the one hand and $f_{i,start}$ and $f_{i,end}$ on the other. This reduces the matrix in Equation (110) to a simpler one, for which at least a direct, though cumbersome, expression for the inverse can be computed. However, the residuals for the individual image rows may become rather large. Another obstacle might be that the intercept of the regression line is not close to zero, although this can probably be coped with.

Using dark areas (smear areas) in-flight could make it possible to compare measurement with theory.

22.11 Inter-band gain alignment

Due to small gain drifts in the detector and electronics, the observed charge from two bands of the UVN detector may not align perfectly. The gain alignment correction algorithm provides a correction to align the two bands of a UVN detector. The correction factor might either be a dynamic CKD or a static CKD.

22.11.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	$e^- s^{-1}$
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$e^{-2} s^{-2}$
f_{align}	gain alignment factor	1

22.11.2 Algorithm description

The gain alignment factor holds for all pixels in a band, with the property that the average of the two alignment factors inside the same detector is one.

$$S_o[\mathbf{x}_{img}] = f_{align} \cdot S_i[\mathbf{x}_{img}] \cdot \quad (163)$$

22.11.3 Error propagation

The gain alignment correction is completely correlated with other multiplicative corrections. Therefore the factor itself can be considered to be exact.

$$\sigma_o^2[\mathbf{x}_{img}] = f_{align}^2 \sigma_i^2[\mathbf{x}_{img}] \quad (164)$$

22.12 Exposure time division

The signal is divided by the exposure time. From here on, the signal is expressed in electrons per second. The exposure time is extracted from the engineering. A description of the exposure sequence can be found in section 9.1.5.

22.12.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	$e^- s^{-1}$
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$e^{-2} s^{-2}$
t_{exp}	exposure time, excluding frame transfer time	s

22.12.2 Algorithm description

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}]/t_{\text{exp}} \cdot \quad (165)$$

Note that the exposure time does not include the frame transfer time.

22.12.3 Error propagation

The exposure time is expected to be known exactly:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}]/t_{\text{exp}}^2 \cdot \quad (166)$$

22.13 Pixel response non-uniformity

Pixel response non-uniformity (PRNU) means that different pixels in a detector do not have the same quantum efficiency. This is mainly caused by manufacturing aspects such as differing pixel sizes and detector surface treatment. The PRNU results in an image that has small variations from pixel to pixel. This high-frequency variation is in the order of one percent.

For the calibration of PRNU, an unbinned WLS/LED/DLED measurement is smoothed and divided, pixel-wise, by the original measurement. This factor forms the PRNU CKD. The smoothing operation consists of several steps; for details we refer to the algorithm theoretical basis document for TROPOMI UVN on-ground calibration key data calculation [RD11].

This algorithm applies only to UVN. It is related to Equation (14) in the forward model part. In the SWIR case, any PRNU effect should already have been incorporated in the pixel-dependent non-linearity.

22.13.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$e^- s^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$e^{-2} s^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	$e^- s^{-1}$
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$e^{-2} s^{-2}$
$c_{\text{prnu}}[\mathbf{x}_{\text{det}}]$	PRNU factor	1
$s_{\text{prnu}}^2[\mathbf{x}_{\text{det}}]$	variance of PRNU factor	1

22.13.2 Algorithm description

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] \frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} c_{\text{prnu}}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \cdot \quad (167)$$

Here, c_{prnu} is the ratio between the smoothed and the original calibration measurement. A ratio smaller than 1 implies a local peak in the response; this local peak is therefore negated in the processing algorithm step.

22.13.3 Error propagation

The error will be adjusted according to

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \left(\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} c_{\text{prnu}}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + \overline{s_{\text{prnu}}^2[\mathbf{x}_{\text{det}}]} S_i[\mathbf{x}_{\text{img}}]^2 \cdot \quad (168)$$

Note that the error in the PRNU correction is propagated directly using the product rule of the formal error propagation mechanism. Here we make use of the definition of the mean unbinned variance described in Section 20.4.2.

23 SWIR specific corrections

In the following sections, algorithms that apply only to the SWIR module are described, as shown in Figure 48. This accounts for Bands 7 and 8.

Since in the SWIR detector no binning takes place, the distinction between the image coordinate system and the detector coordinate system vanishes. In particular, that means that the symbols \mathbf{x}_{img} and \mathbf{x}_{det} are completely interchangeable. Although the physics behind an algorithm can make a choice for either \mathbf{x}_{img} or \mathbf{x}_{det} notation more appropriate, we will only use the former.

23.1 ADC conversion

The SWIR detector has four ADCs. The analogue signals are read out by the 14-bit ADCs and thereby converted into digital numbers. Here in the reverse algorithm the signal is converted into Volts; for each ADC a conversion factor has been set. The ADC introduces a non-linearity; this can be described by an additive non-linearity function that translates the original signal (in DN) to the corrected signal (also in DN). Afterwards the conversion as described above can be applied. An obstacle in using a non-linearity function is that it has to be applied to the co-added signals that constitute the measured signal. The fact that this data is difficult to retrieve means that it will increase the variance of the propagated signal. However, this objection only holds near non-smooth parts of the non-linearity function. This algorithm is related to Equation (25) in the forward model part.

23.1.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	DN
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	DN ²
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	V
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	V ²
$a[\mathbf{x}_{\text{img}}]$	ADC identifier associated with an image pixel	1
$f_{a,\text{dn2v}}$	unit conversion factor, per ADC	V DN ⁻¹
$g_{a,\text{nl}}(S_i[\mathbf{x}_{\text{img}}])$	ADC non-linearity correction, per ADC a	1
$s_{a,\text{nl}}^2(S_i[\mathbf{x}_{\text{img}}])$	variance of the ADC non-linearity correction, per ADC	1

23.1.2 Algorithm description

As described above, the ADC conversion factor is applied on the input signal that has been corrected for non-linearity as an intermediate step. The nonlinearity function is implemented as a look-up table, from the signal in (integer) DN to an additive term in (real-valued) DN. Table values can show rather discontinuous behavior from one signal value to the next. If $N_{\text{coadd}} > 1$, the input signal is generally not an integer. The nonlinearity table value belonging to the nearest integer signal is used in that case.

Note that each pixel can be associated with a particular ADC, and each ADC has its own unit conversion factor and non-linearity correction table. We use $a[\mathbf{x}_{\text{img}}]$ as the ADC identifier associated with a pixel, and the subscript a in the variables f and g .

$$S_o[\mathbf{x}_{\text{img}}] = f_{a,\text{dn2v}} (S_i[\mathbf{x}_{\text{img}}] + g_{a,\text{nl}}(\text{round}(S_i[\mathbf{x}_{\text{img}}]))) . \quad (169)$$

23.1.3 Error propagation

The ADC conversion factor f_{dn2v} is set pre-flight and contains no errors. The non-linearity function, when added, will hardly change the magnitude of the signal; we can therefore safely assume that $d(S_i + g_{a,\text{nl}})/dS_i = 1$. Therefore the effect of any non-linearity on the error propagation is limited to an extra term $s_{\text{nl}}^2(S_i[\mathbf{x}_{\text{img}}])$. This term is also implemented as a look-up table with integer signal values as indices.

An important error source related to a non-linearity function is the fact that the function argument is a co-added signal, not the original signals per frame. In other algorithms, this behavior is expressed in the error term s_{coadd}^2 . We refer to Section 22.4.3 for an example. However, due to the discontinuous behavior of the

nonlinearity function itself, the error magnitude is hard to quantify. In particular, in the case without co-additions, the signal contains no noise and the resulting error is expected to be low. On the other hand, for $N_{\text{coadd}} > 1$, a signal value near a 'jump' makes the nonlinearity quite uncertain. The choice has been made to include this uncertainty in the overall error term s_{nlm}^2 . The error propagation is therefore

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = f_{a,\text{dn}2v}^2 \{ \sigma_i^2[\mathbf{x}_{\text{img}}] + s_{a,\text{nlm}}^2(\text{round}(S_i[\mathbf{x}_{\text{img}}])) \} . \quad (170)$$

23.1.4 Remark

The original, not co-added, pixel data can in theory be approximated using small-pixel column scaling. However, the higher noise of small-pixel columns, together with inevitable reconstruction errors, will negate the possible accuracy of the non-linearity function applied to the reconstructed pixels per frame. Therefore such a strategy will not be pursued.

23.2 Memory effect correction

The memory effect is related to Section 17.2 in the forward model part. This effect occurs when the read-out of a detector affects the next read-out. In the case of the SWIR detector, the hysteresis or memory effect scales with the difference in signal level between the current and previous read-outs. This means that when a pixel increases in intensity between two consecutive frames the memory effect causes the intensity in the pixel to be too low. However, if the intensity decreases between two frames the memory effect causes the intensity to be too high. Measurements have shown that the relative memory effect depends on the jump in signal. The effect is mainly linearly related to the jump size. However, a small second order effect is also visible. The memory effect leads to diffusion: the signal becomes smoother in the temporal direction. Our current understanding of the forward model indicates that the signal change is completely determined by the difference of the current frame and the previous frame, even (if the current frame is the first of a co-addition series) if the previous frame belongs to the previous image. Note further that this previous frame has already been affected by the effect.

Consider the assumption that the memory effect is the same for positive and negative jumps between frames. Then the signal between frames 2 and N_{coadd} is only shifted. These frames give the same contribution to the co-added signal. The co-added signal only changes because of a memory effect working on the first frame. Conservation of signal is achieved in the long term. Under this assumption, complete knowledge of the last frame of each co-added image is sufficient for a complete reconstruction in a correction algorithm.

However, the memory effect is not symmetric concerning jump signs (see below); this makes the effect harder to correct.

We define the signal jump $\Delta(S)$ as

$$\Delta(S) = S_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, k] - S_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, k-1] \quad 2 \leq k \leq N_{\text{coadd}} , \quad (171a)$$

$$\Delta(S) = S_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, 1] - S_{\text{exp},i}[\mathbf{x}_{\text{img}}, j-1, N_{\text{coadd}}] \quad k = 1 . \quad (171b)$$

Here the $S_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, k]$ denotes the k -th co-addition of time step j .

The memory effect causes the signal to change:

$$S'_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, k] = S_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, k] + f(\Delta(S)) \quad (172)$$

Here f is almost a linear function $f = c\Delta$; the constant c is approximately

$$c = \begin{cases} -0.016 & \text{if } \Delta(S) < 0 \\ -0.019 & \text{otherwise.} \end{cases} \quad (173)$$

23.2.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$ ($= S_i[\mathbf{x}_{\text{img}}, j]$)	signal in image pixel \mathbf{x}_{img} (at current time step) before correction	V
$S_i[\mathbf{x}_{\text{img}}, j - 1]$	signal in image pixel \mathbf{x}_{img} at previous time step before correction	V
$\sigma_i^2[\mathbf{x}_{\text{img}}, j]$	signal variance in image pixel \mathbf{x}_{img} at current time step before correction	V ²
$\sigma_i^2[\mathbf{x}_{\text{img}}, j - 1]$	signal variance in image pixel \mathbf{x}_{img} at previous time step before correction	V ²
$S_o[\mathbf{x}_{\text{img}}]$ ($= S_o[\mathbf{x}_{\text{img}}, j]$)	signal in image pixel \mathbf{x}_{img} (at current time step) after correction	V
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	V ²
N_{coadd}	number of co-additions	1
$S_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, k]$	original signal of co-addition k at time step j	V
$S'_{\text{exp},i}[\mathbf{x}_{\text{img}}, j, k]$	signal, after memory effect, of co-addition k at time step j	V
$s_{\text{res}}^2[\mathbf{x}_{\text{img}}]$	residual signal variance term in image pixel \mathbf{x}_{img}	V ²
$p_{1,\text{pos}}[\mathbf{x}_{\text{img}}]; p_{1,\text{neg}}[\mathbf{x}_{\text{img}}]$	linear coefficient in case of positive / negative signal jump	1
$p_{2,\text{pos}}[\mathbf{x}_{\text{img}}]; p_{2,\text{neg}}[\mathbf{x}_{\text{img}}]$	quadratic coefficient in case of positive / negative signal jump	V ⁻¹
$s_{p,1,\text{pos}}^2[\mathbf{x}_{\text{img}}]; s_{p,1,\text{neg}}^2[\mathbf{x}_{\text{img}}]$	variance of linear coefficient for both signal jump signs	1
$s_{p,2,\text{pos}}^2[\mathbf{x}_{\text{img}}]; s_{p,2,\text{neg}}^2[\mathbf{x}_{\text{img}}]$	variance of quadratic coefficient for both signal jump signs	V ⁻²

23.2.2 Algorithm description

The reverse model consists of extracting S from S' . Rewriting Equation (171a) gives $S_{\text{exp},i} = S'_{\text{exp},i} - f(\Delta(S))$ where the Δ consists of two terms that are still unknown. We make a small error if we use the difference of the signal after the memory effect:

$$S_{\text{exp},i} \approx S'_{\text{exp},i} - f(\Delta(S')) \quad (174)$$

This simplified reverse algorithm can be replaced by a more sophisticated one by constructing an inverse like in the smear correction algorithm (provided that f is at most a linear function); in fact that means solving for the unknown terms on the right-hand side. Since f contains a quadratic term the inverse will be hard to compute. However, this sophisticated approach is not considered necessary here since this extra correction scales with c^2 . Therefore we stay with the approximated equation 174.

Because small pixel data (i.e. the original images that constitute a co-added signal) is not available, the reverse model approximated in terms of the co-added signal would be

$$S_o[\mathbf{x}_{\text{img}}, j] = S_i[\mathbf{x}_{\text{img}}, j] + \frac{1}{N_{\text{coadd}}} f(\Delta), \quad (175)$$

$$\Delta = (S_i[\mathbf{x}_{\text{img}}, j] - S_i[\mathbf{x}_{\text{img}}, j - 1]).$$

It can be shown that this correction algorithm gives large over-corrections in some cases. Therefore, small-pixel information (possibly the last small-pixel signal of each image) would have to be included.

Concerns about the reliability of small-pixel column scaling (see Appendix B), together with the consideration that the large majority of images will, with our current understanding, only negligibly be affected by temporal signal shifts due to the memory effect, lead to the decision not to implement a memory effect correction algorithm for $N_{\text{coadd}} > 1$.

For $N_{\text{coadd}} = 1$ we have:

$$S_o[\mathbf{x}_{\text{img}}, j] = S_i[\mathbf{x}_{\text{img}}, j] - f(\Delta),$$

$$\Delta = (S_i[\mathbf{x}_{\text{img}}, j] - S_i[\mathbf{x}_{\text{img}}, j - 1]),$$

$$f(\Delta) = \begin{cases} p_{1,\text{pos}}[\mathbf{x}_{\text{img}}]\Delta + p_{2,\text{pos}}[\mathbf{x}_{\text{img}}]\Delta^2 & \text{if } \Delta > 0, \\ p_{1,\text{neg}}[\mathbf{x}_{\text{img}}]\Delta + p_{2,\text{neg}}[\mathbf{x}_{\text{img}}]\Delta^2 & \text{if } \Delta < 0. \end{cases} \quad (176)$$

For the first measurement ($j = 0$) in a continuous measurement series, the previous measurement is unknown or irrelevant and therefore no correction can be imposed.

23.2.3 Error propagation

Because the memory effect is part of our model, we have to describe the evolution of the error even if no action is taken. Therefore, for $N_{\text{coadd}} > 1$ we set

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] + f\left(\frac{S_i[\mathbf{x}_{\text{img}}, j] - S_i[\mathbf{x}_{\text{img}}, j-1]}{N_{\text{coadd}}}\right)^2. \quad (177)$$

That is, the error is associated directly with a correction with step size Δ/N_{coadd} .

For $N_{\text{coadd}} = 1$ (and $j \neq 0$) we use formal error propagation, but allow for a residual extra error term s_{res}^2 :

$$\begin{aligned} \sigma_o^2[\mathbf{x}_{\text{img}}] = & \{1 - p_1[\mathbf{x}_{\text{img}}] - 2p_2[\mathbf{x}_{\text{img}}]\Delta\}^2 \sigma_i^2[\mathbf{x}_{\text{img}}, j] \\ & + \{p_1[\mathbf{x}_{\text{img}}] + 2p_2[\mathbf{x}_{\text{img}}]\Delta\}^2 \sigma_i^2[\mathbf{x}_{\text{img}}, j-1] \\ & + \Delta^2 s_{p,1}^2[\mathbf{x}_{\text{img}}] + \Delta^4 s_{p,2}^2[\mathbf{x}_{\text{img}}] + s_{\text{res}}^2[\mathbf{x}_{\text{img}}] \end{aligned} \quad (178)$$

Here we assume that the correlation between p_1 and p_2 is negligible (if not, this term can always be lumped towards s_{res}^2).

23.3 Artifact correction

For exposure times below 81.92 ms, the SWIR detector shows multiple detector read-out interference artifacts. They can more or less be classified as the horizontal (i.e. row), the vertical (i.e. column), the end-of-readout, and very short exposure artifacts. All artifacts are assumed to affect the analogue offset, without affecting the exposure time dependent part of the signal.

All these artifacts can be modeled, although this is difficult and for some exposure times additional artifacts can be observed in some parts of the detector. Therefore it has been decided to describe the total artifact effect as a pixel map. For each value of the engineering parameter t_{intdelay} of the image after the current image, the artifact is uniquely defined. Since exposure times below 81.92 ms are not used in-flight, we know beforehand the limited set of different t_{intdelay} and can produce a corresponding set of artifact maps. The restriction is that the last (possibly co-added) image of a measurement series must be discarded if the value of t_{intdelay} changes; this is the responsibility of the user.

23.3.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	V
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	V ²
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	V
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	V ²
t_{intdelay}	engineering parameter	s
$O_{\text{art}}[\mathbf{x}_{\text{img}}, t_{\text{intdelay}}]$	artifact correction	V
$s_{\text{art}}^2[\mathbf{x}_{\text{img}}, t_{\text{intdelay}}]$	variance of artifact correction	V ²

23.3.2 Algorithm description

The artifact correction is applied to the input signal:

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] - O_{\text{art}}[\mathbf{x}_{\text{img}}, t_{\text{intdelay}}]. \quad (179)$$

Note that the artifact is pixel-dependent. No other dependencies, such as on temperature, are envisaged.

23.3.3 Error propagation

The error is propagated using the standard rules:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] + s_{\text{art}}^2[\mathbf{x}_{\text{img}}, t_{\text{intdelay}}]. \quad (180)$$

23.4 Analog offset correction

Before digitization by the ADC, an offset voltage is added to the amplified detector pixel voltage, in order to prevent negative voltages to be digitized. Moreover, within the FEE another offset is added to achieve a more optimal voltage signal range. The reverse model corrects these two offsets using one combined offset correction.

This algorithm is related to Section 18.2 in the forward model chapter.

23.4.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	V
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	V ²
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	V
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	V ²
$O_{\text{cmos}}[\mathbf{x}_{\text{img}}]$	analog offset correction	V
$s_{O_{\text{cmos}}}^2[\mathbf{x}_{\text{img}}]$	variance of analog offset correction	V ²

23.4.2 Algorithm description

The combined offset correction is applied to the input signal:

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] - O_{\text{cmos}}[\mathbf{x}_{\text{img}}] . \quad (181)$$

Note that the offset is pixel-dependent. No other dependencies are envisaged. In particular, the offset will not be considered temperature-dependent since the detector temperature is stabilized to a high degree. However, when the temperature set point changes, an adjusted offset CKD will be provided.

23.4.3 Error propagation

The error is propagated using the standard rules:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] + s_{O_{\text{cmos}}}^2[\mathbf{x}_{\text{img}}] . \quad (182)$$

23.5 Conversion from voltage to charge

The signal in forward direction is converted from charge to voltage. Therefore, in the reverse model, the inverse conversion takes place. The conversion, however, is not entirely linear as function of the signal. This non-linear behavior will be separately addressed, and corrected for, in the next section.

This algorithm is related to Section 18.1 in the forward model part.

23.5.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	V
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	V ²
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e ⁻
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e ⁻²
$a[\mathbf{x}_{\text{img}}]$	ADC identifier associated with an image pixel	1
$f_{\sqrt{2e}}(a[\mathbf{x}_{\text{img}}])$	unit conversion factor, per ADC	e ⁻ V ⁻¹
$s_{\sqrt{2e}}^2(a[\mathbf{x}_{\text{img}}])$	uncertainty of the unit conversion factor, per ADC	e ⁻² V ⁻²

23.5.2 Algorithm description

Each detector pixel can be associated with a particular ADC, and each ADC has its own voltage-to-charge conversion factor.

$$S_o[\mathbf{x}_{\text{img}}] = f_{v2e}(a[\mathbf{x}_{\text{img}}]) S_i[\mathbf{x}_{\text{img}}] , \quad (183)$$

23.5.3 Error propagation

Although this conversion factor is correlated to other multiplicative factors further downstream in the processing flow, error propagation takes the uncertainty of f_{adc} into account here. Later on, the correlation in the error will be corrected for.

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = f_{v2e}^2(a[\mathbf{x}_{\text{img}}]) \sigma_i^2[\mathbf{x}_{\text{img}}] + s_{v2e}^2(a[\mathbf{x}_{\text{img}}]) S_i[\mathbf{x}_{\text{img}}]^2 . \quad (184)$$

23.6 Amplifier non-linearity correction

This correction has been removed for the time being since no accurate CKD could be established.

23.7 Dark current correction

During the exposure, the detector gathers additional signal that does not come from the source under consideration, but is intrinsic to the direct environment of the detector. This dark flux signal is here defined as that part of the signal that is not intrinsic to the source, and scales with the exposure time t_{exp} . Not included is straylight, which is corrected for in a separate step.

The dark flux signal is described as the sum of the detector dark current and the thermal background. These parts of the dark flux are corrected separately, although the order of these corrections can be interchanged. In this section we will describe the dark current; thermal background correction is explained in section 23.8.

The correction is applied for each pixel \mathbf{x}_{img} separately.
 This algorithm is related to Section 17.1 in the forward model part.

23.7.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
t_{exp}	exposure time	s
$S_{\text{dark}}[\mathbf{x}_{\text{img}}]$	dark flux signal in image pixel \mathbf{x}_{img}	e^-
$F_{\text{dc}}[\mathbf{x}_{\text{img}}]$	dark current flux	e^-s^{-1}
$F_{\text{therm}}[\mathbf{x}_{\text{img}}]$	thermal background flux	e^-s^{-1}
$F_{\text{dc},0}[\mathbf{x}_{\text{img}}]$	long term (i.e. orbits to days) dark current	e^-s^{-1}
$s_{\text{dc},0}^2[\mathbf{x}_{\text{img}}]$	variance of long term (i.e. orbits to days) dark current	$e^{-2}s^{-2}$
$F_{\text{dc},\text{rts}}[\mathbf{x}_{\text{img}}]$	dark current because of random telegraph signal	e^-s^{-1}
$s_{\text{dc},\text{rts}}^2[\mathbf{x}_{\text{img}}]$	additional error term due to RTS	$e^{-2}s^{-2}$
$F_{\text{dc},T}[\mathbf{x}_{\text{img}}]$	temperature-dependent dark current	e^-s^{-1}
T_{det}	detector temperature	K
$T_{0,\text{det}}$	detector reference temperature	K
$D_{T,\text{det}}[\mathbf{x}_{\text{img}}]$	detector temperature dependence	$e^-s^{-1}K^{-1}$
$s_{D,T,\text{det}}^2[\mathbf{x}_{\text{img}}]$	variance of detector temperature dependence	$e^{-2}s^{-2}K^{-2}$

23.7.2 Algorithm description

We begin with stating that the dark flux consists of a dark current flux and a thermal background flux:

$$S_{\text{dark}}[\mathbf{x}_{\text{img}}] = t_{\text{exp}} (F_{\text{dc}}[\mathbf{x}_{\text{img}}] + F_{\text{therm}}[\mathbf{x}_{\text{img}}]) . \quad (185)$$

The dark current contribution F_{dc} consists of three terms, with a constant component $F_{\text{dc},0}$ that is typically determined over a timescale of several orbits to days, and two variable components that are caused by random telegraph signal and temperature dependence. Detector pixels affected by RTS exhibit a time-dependent dark current component that may jump between multiple discrete levels at timescales from shorter than t_{int} to longer than the orbital time. Pixels may develop RTS behavior over time, usually after suffering the impact of a high energy particle, and may recover from as the result of (partial) annealing of the detector. RTS pixels are flagged in the pixel quality flagging step. The current baseline is that we flag the RTS pixels and do not try to correct them here. However, an RTS error will be added to the error propagation, see [RD12]. In addition, dark current exhibits an orbital dependence $F_{\text{dc},T}[\mathbf{x}_{\text{img}}]$ because of detector temperature variations. Since the detector temperature will be stabilized, a first-order approximation will suffice:

$$F_{\text{dc},T}[\mathbf{x}_{\text{img}}] = (T_{\text{det}} - T_{0,\text{det}}) D_{T,\text{det}}[\mathbf{x}_{\text{img}}] . \quad (186)$$

Thus, dark current can be described as the sum of three components:

$$F_{\text{dc}} = F_{\text{dc},0}[\mathbf{x}_{\text{img}}] + F_{\text{dc},\text{rts}}[\mathbf{x}_{\text{img}}] + F_{\text{dc},T}[\mathbf{x}_{\text{img}}] . \quad (187)$$

where the RTS component will be ignored.

The dark current correction algorithm consists of the subtraction of the signal by the dark current signal as defined in the equations above:

$$\begin{aligned} S_o[\mathbf{x}_{\text{img}}] &= S_i[\mathbf{x}_{\text{img}}] - t_{\text{exp}} (F_{\text{dc}}[\mathbf{x}_{\text{img}}]) \\ &= S_i[\mathbf{x}_{\text{img}}] - t_{\text{exp}} (F_{\text{dc},0}[\mathbf{x}_{\text{img}}] + (T_{\text{det}} - T_{0,\text{det}}) D_{T,\text{det}}[\mathbf{x}_{\text{img}}]) . \end{aligned} \quad (188)$$

The temperature dependency CKDs will be established in-flight.

23.7.3 Error propagation

The formula for the error propagation is obtained using standard rules:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] + t_{\text{exp}}^2 \text{Var} F_{\text{dc}}[\mathbf{x}_{\text{img}}] , \quad (189)$$

where

$$\text{Var} F_{\text{dc}}[\mathbf{x}_{\text{img}}] = s_{\text{dc},0}^2[\mathbf{x}_{\text{img}}] + s_{\text{dc},\text{rts}}^2[\mathbf{x}_{\text{img}}] + (T_{\text{det}} - T_{0,\text{det}})^2 s_{D,T,\text{det}}^2[\mathbf{x}_{\text{img}}] \quad (190)$$

23.8 Thermal background correction

During the exposure, the detector gathers additional signal that does not come from the source under consideration, but is intrinsic to the direct environment of the detector. This dark flux signal is here defined as that part of the signal that is not intrinsic to the source, and scales with the exposure time t_{exp} . Not included is straylight, which is corrected for in a separate step.

The dark flux signal is described as the sum of the detector dark current and the thermal background. These parts of the dark flux are corrected separately, although the order of these corrections can be interchanged. In this section we will describe the thermal background; dark current correction is explained in section 23.7

This algorithm is related to Section 17.1 in the forward model part.

23.8.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
t_{exp}	exposure time	s
$S_{\text{dark}}[\mathbf{x}_{\text{img}}]$	dark flux signal in image pixel \mathbf{x}_{img}	e^-
$F_{\text{dc}}[\mathbf{x}_{\text{img}}]$	dark current flux	$e^{-s^{-1}}$
$F_{\text{therm}}[\mathbf{x}_{\text{img}}]$	thermal background flux	$e^{-s^{-1}}$
$F_{\text{therm},0}$	thermal background flux with nominal QE and ice layer	$e^{-s^{-1}}$
F_0	overall thermal background for thermally nominal conditions	$e^{-s^{-1}}$
$s_{F,0}^2$	variance of this thermal background signal	$e^{-2}s^{-2}$
T_{det}	detector temperature	K
T_{obm}	optical bench temperature	K
T_{cu}	calibration unit temperature	K
$T_{0,\text{det}}$	detector reference temperature	K
$T_{0,\text{obm}}$	optical bench reference temperature	K
$T_{0,\text{cu}}$	calibration unit reference temperature	K
$\mathbf{I}_{\text{cu}}[\text{icid}]$	indicator function; switched on when calibration unit is visible	1
$D_{T,\text{det}}[\mathbf{x}_{\text{img}}]$	detector temperature dependence	$e^{-s^{-1}}K^{-1}$
$D_{T,\text{obm}}$	optical bench temperature dependence	$e^{-s^{-1}}K^{-1}$
$D_{T,\text{cu}}$	calibration unit temperature dependence	$e^{-s^{-1}}K^{-1}$
$s_{D,T,\text{det}}^2[\mathbf{x}_{\text{img}}]$	variance of detector temperature dependence	$e^{-2}s^{-2}K^{-2}$
$s_{D,T,\text{obm}}^2$	variance of optical bench temperature dependence	$e^{-2}s^{-2}K^{-2}$
$s_{D,T,\text{cu}}^2$	variance of calibration unit temperature dependence	$e^{-2}s^{-2}K^{-2}$
Q	differential quantum efficiency	1
D_Q	temperature dependence of Q	K^{-1}
$s_{D,Q}^2$	variance of temperature dependence of Q	K^{-2}

23.8.2 Algorithm description

We begin with stating that the dark flux consists of a dark current flux and a thermal background flux, of which the latter is elaborated on in this section:

$$S_{\text{dark}}[\mathbf{x}_{\text{img}}] = t_{\text{exp}} (F_{\text{dc}}[\mathbf{x}_{\text{img}}] + F_{\text{therm}}[\mathbf{x}_{\text{img}}]) . \quad (191)$$

The thermal background signal, which is defined per pixel, depends on the thermal surroundings of the detector. The surroundings are approximated by the temperatures of the optical bench module T_{obm} , the calibration unit T_{cu} , and the immersed grating T_{ig} . The last component will be ignored since the immersed grating temperature is assumed to have the same temperature as the OBM.

All temperatures are stabilized and first-order approximations are used. The calibration unit term may not be present: when the folding mirror in the UVN bench allows the view to exit the instrument, the calibration unit is not visible and its thermal background is not present. This will be implemented as a switch that is on or off depending on the type of measurement.

The light sources within the calibration unit are cold enough to ignore the history of the CU.

The measured thermal background signal is affected by any optical effects and detector effects before it is recorded as an electronic signal. A change in detector temperature will also impact the quantum efficiency of the detector and hence also its sensitivity to the thermal background radiation. To account for this a correction

term called the differential quantum efficiency Q is implemented when estimating the total thermal background flux. The differential quantum efficiency is described by

$$Q = (T_{\text{det}} - T_{0,\text{det}}) D_Q, \quad (192)$$

where D_Q describes the sensitivity of the detector to temperature variations of the quantum efficiency. The total thermal background flux is therefore

$$\begin{aligned} F_{\text{therm}} &= (1 + Q) F_{\text{therm},0} \\ &= (1 + Q) [F_0 + (T_{\text{obm}} - T_{0,\text{obm}}) D_{T,\text{obm}} + \mathbf{I}_{\text{cu}}[\text{icid}](T_{\text{cu}} - T_{0,\text{cu}}) D_{T,\text{cu}}], \end{aligned} \quad (193)$$

where the conventions for first-order approximations are similar as in Equation (186).

The thermal background correction algorithm consists of the subtraction of the signal by the thermal background signal as defined in the equations above:

$$\begin{aligned} S_o[\mathbf{x}_{\text{img}}] &= S_i[\mathbf{x}_{\text{img}}] - t_{\text{exp}} F_{\text{therm}} \\ &= S_i[\mathbf{x}_{\text{img}}] - t_{\text{exp}} (1 + Q) \{ F_0 + (T_{\text{obm}} - T_{0,\text{obm}}) D_{T,\text{obm}} + \mathbf{I}_{\text{cu}}[\text{icid}](T_{\text{cu}} - T_{0,\text{cu}}) D_{T,\text{cu}} \}. \end{aligned} \quad (194)$$

The temperature dependency CKDs will be established in-flight. Although it is expected that the temperature sensors on OBM and CU are representative, the occurrence of thermal gradient, and given that emission scales with T^4 , average emission can be higher than expected from average temperature. Because of these orbital temperature gradients, the temperature dependencies D_T may be more a function of orbit phase than of temperature sensor reading.

23.8.3 Error propagation

The formula for the error propagation is obtained using standard rules:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \sigma_i^2[\mathbf{x}_{\text{img}}] + t_{\text{exp}}^2 \text{Var} F_{\text{therm}}, \quad (195)$$

where

$$\begin{aligned} \text{Var} F_{\text{therm}} &= F_{\text{therm},0}^2 (T_{\text{det}} - T_{0,\text{det}})^2 s_{D,QE}^2 \\ &+ (1 + Q)^2 (s_{F,0}^2 + (T_{\text{obm}} - T_{0,\text{obm}})^2 s_{D,T,\text{obm}}^2 \\ &+ \mathbf{I}_{\text{cu}}[\text{icid}](T_{\text{cu}} - T_{0,\text{cu}})^2 s_{D,T,\text{cu}}^2). \end{aligned} \quad (196)$$

The errors in the temperature dependencies of the optical bench module and the calibration unit are neglected, because these errors are expected to be very small.

23.9 Residual correction

Apart from the actual illuminated signal, the signal recorded by the SWIR detector consists of a number of additional components. These components, all additive, need to be corrected for in the L01b Processor. We have already discussed the offset (Section 23.4) and the dark flux (Section 23.7). Measurements without illumination, the so-called background measurements, contain only a few of these additive components. At this stage in the L01b Processor, with the offset and the dark flux already having been coped with, the background images (now renamed residual images) contain only unmodeled artifacts like electromagnetic compatibility (EMC). Note that the residual is defined per ICID and cannot be described in a more general way such as the dark current (which can be modeled as a flux).

In the residual correction algorithm, illuminated images are corrected with the aggregated residual signal of their associated ICID. The residual aggregate has already been described for UVN (Section 22.8); for the SWIR detector, the algorithm is exactly the same. If the aggregated residual is not available, a fallback strategy is to use the residual CKD. This CKD has been constructed in the same way as the residual aggregate, and will be of high quality (concerning, for example, the signal-to-noise ratio) but has probably not been collected close in time as the illuminated images. The residual CKD contains per definition no noise; this has been

incorporated in its error. After the residual subtraction, the error due to the offset should have disappeared. EMC, if it occurs, is a known unknown that is exactly the same for both illuminated and dark image. Hence this term, no matter its contribution, cancels as well due to the residual correction. This algorithm is related to Section 17.1 in the forward model part.

23.9.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	e^-
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	e^{-2}
$S_{res}[\mathbf{x}_{img}]$	residual aggregate signal	e^-
$s_{res}^2[\mathbf{x}_{img}]$	variance (error) of residual aggregate signal	e^{-2}
$s_{\mu,res}^2$	offset variance propagated to this algorithm step	e^{-2}
$\sigma_{i,red}^2$	propagated error without offset contribution	e^{-2}

23.9.2 Algorithm description

The residual signal is subtracted from the current signal:

$$S_o[\mathbf{x}_{img}] = S_i[\mathbf{x}_{img}] - S_{res}[\mathbf{x}_{img}] . \quad (197)$$

23.9.3 Error propagation

An interesting aspect of the residual subtraction is that it may have, at least partly, an ameliorating effect on the error: The error on the offset subtraction cancels out if the offset does not depend on the temperature. Contrary to UVN, it is not likely that (part of) the dark flux error will cancel: because of the temperature differences, correlations between dark flux components in illuminated and dark measurements are low. The (pixel-dependent) offset error term has been introduced as $s_{O_{cmos}}^2[\mathbf{x}_{img}]$ in Section 23.4 and has been propagated ever since. The total propagation effect is multiplicative; that is, the original offset variance has been evolved towards $s_{\mu,res}^2$. If a significant dependence of the offset on the temperature exists, however, then our assumption is not valid and we have to set $s_{\mu,res}^2 = 0$. The variance of the residual signal can immediately be applied:

$$\sigma_o^2[\mathbf{x}_{img}] = \sigma_i^2[\mathbf{x}_{img}] - s_{\mu,res}^2[\mathbf{x}_{img}] + s_{res}^2[\mathbf{x}_{img}] . \quad (198)$$

A far better alternative than this bookkeeping is to skip the error propagation for the offset (giving the smaller error $\sigma_{i,red}^2$ instead of σ_i^2) if beforehand is known that the signal will be processed up to and including the residual correction algorithm. In that case, we simply have

$$\sigma_o^2[\mathbf{x}_{img}] = \sigma_{i,red}^2[\mathbf{x}_{img}] + s_{res}^2[\mathbf{x}_{img}] . \quad (199)$$

23.10 Exposure time division

The signal is divided by the exposure time. From here on, the signal is expressed in electrons per second. The actual exposure time needs to be computed from engineering. An explanation how the exposure time is calculated can be found in section 9.2.4.

23.10.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	e^-
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	e^{-2}
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	$e^- s^{-1}$
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$e^{-2} s^{-2}$
t_{exp}	exposure time	s

23.10.2 Algorithm description

The exposure time is calculated from the engineering parameters as described in section 9.2.4 In the L01b Processor, it is required that the exposure time is at least 82 ms.

Then the signal is divided by the exposure time:

$$S_o[\mathbf{x}_{img}] = \frac{S_i[\mathbf{x}_{img}]}{t_{exp}} . \quad (200)$$

Note that this definition of the exposure time holds at all stages of the L01b Processor.

23.10.3 Error propagation

The exposure time is expected to be known exactly.

$$\sigma_o^2[\mathbf{x}_{img}] = \frac{1}{t_{exp}^2} \sigma_i^2[\mathbf{x}_{img}] . \quad (201)$$

24 Generic corrections II

In this section we describe the generic corrections (i.e. valid for both UVN and SWIR) at the end of the processing flow, as shown in Figure 46.

24.1 Straylight

As described in Sections 10 and 16.3, a detector of the TROPOMI instrument detects both a useful (intended) signal and a straylight (unintended) signal. The purpose of the straylight correction algorithm is to correct the output of the detector for the straylight signal. This algorithm is related to Section 16.3 in the forward model part. We first explain the theory of the so-called matrix multiplication correction algorithm. After that, a practical implementation of this algorithm is given. Then, an alternative correction, the so-called convolution algorithm, will be presented.

In a later stage, a re-assessment was needed concerning out-of-spectral band straylight. Analysis of on-ground measurements showed that for the NIR-detector, straylight from outside the spectral range of this detector was of a magnitude that was considered too high. Since the wavelength immediately outside the NIR detector are not measured by other TROPOMI detectors, a possible correction was not possible within the established correction algorithm. Therefore, an additional out-of-band algorithm has been included. The algorithm, that needs information on the spectral density outside the NIR detector, is invoked before the straylight correction algorithm.

24.1.1 Algorithm: theory

A response of a spectrometer to straylight can be characterized by a set of measurements with a collimated and monochromatic beam. In such a measurement, an intended (direct) signal can be separated from an unintended (straylight) signal. Namely, the largest part of the beam is mapped on a small region of the detector in accordance to the optical design. The signal in this region, also known as the direct region or DR, is the direct, intended or properly imaged contribution. Due to scattering, ghosting and diffraction, a small part of the incident beam ends up everywhere else on the detector. This is straylight: an unintended or improperly imaged contribution. Note that there is a straylight contribution in the direct region as well. For a collimated and monochromatic beam, this contribution is normally negligible compared to the direct contribution. With the assumption that we neglect this direct-region straylight, the signal on the detector can be explained as follows: the direct signal is in the DR and the straylight signal is outside the DR, spread over the rest of the detector.

Most importantly, the straylight signal in each pixel is proportional to the direct signal. If the proportionality constant is known for each detector pixel and for all collimated and monochromatic beams that can be imaged on the detector, the detector image can be corrected for the straylight signal. This is the underlying mechanism for the matrix multiplication algorithm.

To illustrate how the algorithm works, we introduce some simplifications. We assume that there is a 1-to-1 correlation between a direction and a wavelength of the incident beam on one side and a pixel number of the detector on the other side. For a collimated and a monochromatic stimulus, this means that the direct

contribution ends up on a single pixel while the straylight is in the rest of the pixels. The signal on the detector, $S_{\text{psf}}[r, c, r_{\text{stim}}, c_{\text{stim}}]$, is the point spread function (PSF) of the system and can be written as:

$$S_{\text{psf}}[r, c, r_{\text{stim}}, c_{\text{stim}}] = \begin{cases} S_{\text{dpsf}}[r, c, r_{\text{stim}}, c_{\text{stim}}] & \text{for } [r, c] = [r_{\text{stim}}, c_{\text{stim}}] , \\ S_{\text{slpsf}}[r, c, r_{\text{stim}}, c_{\text{stim}}] & \text{for } [r, c] \neq [r_{\text{stim}}, c_{\text{stim}}] , \end{cases} \quad (202)$$

where $[r, c]$ denotes the detector pixel in row r and column c , $[r_{\text{stim}}, c_{\text{stim}}]$ denotes the pixel of the direct region for a collimated and monochromatic stimulus, $S_{\text{dpsf}}[r, c, r_{\text{stim}}, c_{\text{stim}}]$ is the direct point spread function at pixel $[r, c]$ caused by the stimulus at pixel $[r_{\text{stim}}, c_{\text{stim}}]$ and $S_{\text{slpsf}}[r, c, r_{\text{stim}}, c_{\text{stim}}]$ is the straylight point spread function at pixel $[r, c]$ for a stimulus at pixel $[r_{\text{stim}}, c_{\text{stim}}]$. Using the shorthand \mathbf{x} for $[r, c]$, the *relative* straylight response function of the system $M_{\text{SL}}[\mathbf{x}, \mathbf{x}_{\text{stim}}]$ to a stimulus at \mathbf{x}_{stim} can be written as:

$$M_{\text{SL}}[\mathbf{x}, \mathbf{x}_{\text{stim}}] = \begin{cases} 0 & \text{for } \mathbf{x} = \mathbf{x}_{\text{stim}} , \\ \frac{S_{\text{slpsf}}[\mathbf{x}, \mathbf{x}_{\text{stim}}]}{S_{\text{dpsf}}[\mathbf{x}_{\text{stim}}, \mathbf{x}_{\text{stim}}]} & \text{for } \mathbf{x} \neq \mathbf{x}_{\text{stim}} , \end{cases} \quad (203)$$

where $\mathbf{x} = [r, c]$ and $\mathbf{x}_{\text{stim}} = [r_{\text{stim}}, c_{\text{stim}}]$.

To completely characterize the instrument's response to straylight, the relative straylight response function has to be obtained for every \mathbf{x}_{stim} . Each relative straylight response function builds a column of a relative straylight response matrix, $\mathbf{M}_{\text{SL}}[\mathbf{x}, \mathbf{x}_{\text{stim}}]$. If the detector has n rows and m columns, the relative straylight response matrix is a $(n \times m)^2$ matrix and can be written as:

$$\mathbf{M}_{\text{SL}}[r, c, r_{\text{stim}}, c_{\text{stim}}] = \begin{pmatrix} M_{\text{SL}}[0, 0, 0, 0] & M_{\text{SL}}[0, 0, 0, 1] & \dots & M_{\text{SL}}[0, 0, n-1, m-1] \\ M_{\text{SL}}[0, 1, 0, 0] & M_{\text{SL}}[0, 1, 0, 1] & \dots & M_{\text{SL}}[0, 1, n-1, m-1] \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ M_{\text{SL}}[n-1, m-2, 0, 0] & M_{\text{SL}}[n-1, m-2, 0, 1] & \dots & M_{\text{SL}}[n-1, m-2, n-1, m-1] \\ M_{\text{SL}}[n-1, m-1, 0, 0] & M_{\text{SL}}[n-1, m-1, 0, 1] & \dots & M_{\text{SL}}[n-1, m-1, n-1, m-1] \end{pmatrix}. \quad (204)$$

The straylight signal in pixel \mathbf{x} , $S_{\text{stray}}[\mathbf{x}]$, for a broadband source can then be written as:

$$S_{\text{stray}}[\mathbf{x}] = \sum_{\mathbf{x}_{\text{stim}} \in \text{det}} M_{\text{SL}}[\mathbf{x}, \mathbf{x}_{\text{stim}}] S_{\text{direct}}[\mathbf{x}_{\text{stim}}] , \quad (205)$$

where $S_{\text{direct}}[\mathbf{x}_{\text{stim}}]$ is the direct signal in pixel \mathbf{x}_{stim} . The direct signal does not contain straylight and is the unknown to be determined in the algorithm.

Equation (205) is not complete: there are two more contributions to the straylight in pixel \mathbf{x} . One contribution is due to the electromagnetic radiation outside the full field of view of the instrument and the other contribution is due to electromagnetic radiation outside the spectral range of the instrument. In the design phase, efforts are made to reduce these straylight contributions to a negligible level with a proper use of baffles and optical filters. If this is not enough, it is still possible to use the matrix multiplication formalism, but the relative straylight matrix has to be extended to take into account the additional straylight contributions. This will be addressed in Section (24.1.3). For the time being, we will neglect these two straylight contributions.

If straylight signals are represented by the column vector $\mathbf{S}_{\text{stray}}$, Equation (205) can be written in a matrix form:

$$\mathbf{S}_{\text{stray}} = \mathbf{M}_{\text{SL}} \cdot \mathbf{S}_{\text{direct}} , \quad (206)$$

where the column vector $\mathbf{S}_{\text{direct}}$ represents the direct signals. The measured signals, represented by the column vector \mathbf{S}_{meas} , can be written as:

$$\mathbf{S}_{\text{meas}} = \mathbf{S}_{\text{direct}} + \mathbf{M}_{\text{SL}} \cdot \mathbf{S}_{\text{direct}} , \quad (207)$$

The direct signals are given by the subtraction:

$$\mathbf{S}_{\text{direct}} = \mathbf{S}_{\text{meas}} - \mathbf{M}_{\text{SL}} \cdot \mathbf{S}_{\text{direct}} . \quad (208)$$

Finally, we approximate Equation (208) with the following expression:

$$\mathbf{S}_{\text{direct}} \approx \mathbf{S}_{\text{meas}} - \mathbf{M}_{\text{SL}} \cdot \mathbf{S}_{\text{meas}} . \quad (209)$$

The last approximation will only introduce errors of the second order because $\mathbf{S}_{\text{direct}} \approx \mathbf{S}_{\text{meas}}$. This will be discussed in the error propagation section.

Note that it is possible to determine $\mathbf{S}_{\text{direct}}$ without making the approximation $\mathbf{S}_{\text{direct}} \approx \mathbf{S}_{\text{meas}}$ by matrix multiplication of the matrix $(\mathbf{I} + \mathbf{M}_{\text{SL}})^{-1}$ and the vector \mathbf{S}_{meas} . However, this would cause large errors in the practical implementation of the algorithm, as will be discussed below Equation 213.

If the elements of the relative straylight response matrix are known, then the straylight correction is performed by a simple matrix multiplication followed by a simple vector subtraction. Moreover, the matrix \mathbf{M}_{SL} has to be constructed only once provided that the imaging properties of the instrument do not change noticeably. However, the imaging properties of the instrument do change over time and it would be good to find a way to determine how the matrix \mathbf{M}_{SL} evolves with time – the strategy on this has not been decided yet.

In practice, there is not a 1-to-1 correlation between a direction and a wavelength of the incident beam on one side and a pixel number of the detector on the other side. This means that a collimated and a monochromatic stimulus does not illuminate a single pixel on the detector but it illuminates a region on the detector containing several pixels. This region is called the direct region, as discussed before. In reality, it is not possible to measure the direct signal separately from the straylight signal. For this reason, it is practically impossible to exactly determine the borders of the direct region. In practice, we can make an educated guess for the direct region size based on properties of the stimuli and the TROPOMI instrument, and the calibration measurements themselves. This is discussed in [RD11].

For the case that the direct region is larger than one pixel, Equations (204) and (209) can still be used for the straylight correction. However, Equation (203), i.e. the way the elements of the relative straylight response matrix are calculated, needs to be modified slightly:

$$M_{\text{SL}}[\mathbf{x}, \mathbf{x}_{\text{stim}}] = \begin{cases} 0 & \text{for } \mathbf{x} \in \text{DR} , \\ \frac{S_{\text{psf}}[\mathbf{x}, \mathbf{x}_{\text{stim}}]}{\sum_{\mathbf{x} \in \text{DR}} S_{\text{psf}}[\mathbf{x}, \mathbf{x}_{\text{stim}}]} & \text{for } \mathbf{x} \notin \text{DR} . \end{cases} \quad (210)$$

Note that S_{psf} instead of S_{dpsf} is in the denominator. This has been done to emphasize the fact that the direct region has straylight as well. Also note that the pixels on the diagonal of the relative straylight response matrix and their neighboring pixels, all of which correspond to the pixels of the direct regions, are set to zero. An important consequence of this is that the matrix multiplication algorithm does not correct for the straylight in the direct region nor for the aberrations of the instrument.

We have to depart from the approach where a straylight matrix is defined for each pixel, driven by the following considerations:

Memory demands and computational time. A straylight matrix that contains the number of detector pixels squared is clearly not feasible, for both storage space required and computational effort. We can estimate that it is necessary to limit the size of \mathbf{M}_{SL} to a maximum of ca. $(50 \cdot 50) \times (50 \cdot 50)$ per spectrometer.

Calibration time restrictions. If a direct region is comparable to the pixel size, a lot of calibration measurements are needed to cover the whole detector or at least to cover enough conveniently positioned direct regions such that it is possible to interpolate the data points in between. Furthermore, the smaller the direct region size, the lower the signal-to-noise for the measured straylight. This means that long integration times are needed and/or many repeated measurements. All this increases the duration of the straylight calibration campaign.

Reducing the size of the \mathbf{M}_{SL} to 2500×2500 implies the coarsening of the detector image in such a way that the coarse image consists of 50×50 elements, hereafter called blocks. The most important disadvantage of this approach is that it cannot correct sharp straylight features. For a detector size of 1000×1000 , which is a representative detector size for the UVN module, the block size is 20×20 pixels. If we denote signals $\mathbf{S}_{\text{direct,block}}$, $\mathbf{S}_{\text{meas,block}}$ and $\mathbf{S}_{\text{stray,block}}$ as the signals obtained by coarsening the signals $\mathbf{S}_{\text{direct}}$, \mathbf{S}_{meas} and $\mathbf{S}_{\text{stray}}$, respectively, then we could write:

$$\mathbf{S}_{\text{stray,block}} = \mathbf{M}_{\text{SL, reduced}} \cdot \mathbf{S}_{\text{direct,block}} , \quad (211)$$

where $\mathbf{M}_{\text{SL, reduced}}$ is the relative straylight matrix response function for a coarsened detector image; the subscript *reduced* denotes that the size of the matrix is reduced with respect to the original relative straylight response matrix \mathbf{M}_{SL} . The vector representing the straylight signals, $\mathbf{S}_{\text{stray}}$ can be obtained by interpolating the in-between points of $\mathbf{S}_{\text{stray,block}}$:

$$\mathbf{S}_{\text{stray}} = [\mathbf{S}_{\text{stray,block}}]_{\text{expanded}} = [\mathbf{M}_{\text{SL, reduced}} \cdot \mathbf{S}_{\text{direct,block}}]_{\text{expanded}} \approx [\mathbf{M}_{\text{SL, reduced}} \cdot \mathbf{S}_{\text{meas,block}}]_{\text{expanded}} , \quad (212)$$

where the subscript *expanded* denotes the expansion of the vector by interpolation and smoothing. Finally, the direct signals, represented by the vector $\mathbf{S}_{\text{direct}}$, are obtained by a simple vector subtraction:

$$\mathbf{S}_{\text{direct}} = \mathbf{S}_{\text{meas}} - [\mathbf{M}_{\text{SL, reduced}} \cdot \mathbf{S}_{\text{meas, block}}]_{\text{expanded}} \quad (213)$$

By making the approximation $\mathbf{S}_{\text{direct, block}} \approx \mathbf{S}_{\text{meas, block}}$, the coarsening of the measured signal directly influences only the estimate for the straylight contribution. In contrast, if the approximation is not used, the coarsening of the measured signal directly influences also the estimate for the direct signal according to $\mathbf{S}_{\text{direct}} = [(\mathbf{I} + \mathbf{M}_{\text{SL, reduced}})^{-1} \cdot \mathbf{S}_{\text{meas, block}}]_{\text{expanded}}$. Hence, a smaller error is made if we use the approximation that the straylight signal is much smaller than the measured signal.

The matrix coefficients that make a column of the matrix $\mathbf{M}_{\text{SL, reduced}}$ can be obtained from a block detector image (characterization image) in the following way:

$$M_{\text{SL, reduced}}[\mathbf{x}_{\text{block}}, \mathbf{x}_{\text{stim, block}}] = \begin{cases} 0 & \text{for } \mathbf{x}_{\text{block}} \in \text{DR}_{\text{block}} \text{ ,} \\ \frac{S_{\text{block}}[\mathbf{x}_{\text{block}}, \mathbf{x}_{\text{stim, block}}]}{\sum_{\mathbf{x}_{\text{block}} \in \text{DR}_{\text{block}}} S_{\text{block}}[\mathbf{x}_{\text{block}}, \mathbf{x}_{\text{stim, block}}]} & \text{for } \mathbf{x}_{\text{block}} \notin \text{DR}_{\text{block}} \text{ .} \end{cases} \quad (214)$$

where the subscript *block* denotes the block detector image. Note that S_{block} instead of S_{psf} is in the denominator.

How to obtain a block detector image in practice? There are at least two ways. One way uses collimated and monochromatic light beams for straylight characterization measurements. Within this approach, a block detector image can be obtained by summing individual total point spread functions (direct plus straylight contribution) that correspond to individual detector pixels. It is highly unlikely that all total point spread functions can be measured. However, what is not measured can be obtained with interpolation or extrapolation algorithms. The other way for straylight characterization uses light sources with a divergence and a spectral range such to illuminate direct regions that are more or less equal (in size and shape) to that of blocks.

For example, a white light source combined with an optical bandpass filter can illuminate a somewhat rectangular direct region on the detector. The direct region size will depend on the spectral range of the bandpass filter and on the divergence of the source. The direct region shape will *follow* the *smile* of the instrument. In practice, it is easier to match the blocks to the properties of the calibration sources, and not the other way around. Finally, the whole detector surface can be characterized by using different optical filters and rotating the instrument with respect to the source.

24.1.2 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$e^{-} s^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$e^{-2} s^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	$e^{-} s^{-1}$
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$e^{-2} s^{-2}$
$S_{\text{stray}}[\mathbf{x}_{\text{det}}]$	signal only due to straylight in detector pixel \mathbf{x}_{det}	$e^{-} s^{-1}$
$S[\mathbf{x}_{\text{det}}]$	signal in detector pixel \mathbf{x}_{det}	$e^{-} s^{-1}$
$s_{\text{stray}}^2[\mathbf{x}_{\text{det}}]$	variance of signal only due to straylight in detector pixel \mathbf{x}_{det}	$e^{-2} s^{-2}$
M	Size of the straylight matrix; number of blocks	1
M_{det}	Number of blocks from detector pixels	1
M_v	Number of virtual blocks	1
$B[i]$	Block number i	1
\mathbf{B}_{det}	Set of M_{det} blocks	1
$\text{indices}_{\text{interp}}[\mathbf{x}_{\text{det}}]$	Vector with four interpolation indices for detector pixel \mathbf{x}_{det}	1
$\text{coeffs}_{\text{interp}}[\mathbf{x}_{\text{det}}]$	Vector with four interpolation coefficients for detector pixel \mathbf{x}_{det}	1
$\mathbf{S}_{\text{srlf}}[i]$	straylight response function of block i	1
W	size of the first dimension of $\mathbf{S}_{\text{srlf}}[i]$	1
V	size of the second dimension of $\mathbf{S}_{\text{srlf}}[i]$	1
$N_{\text{row, det}}$	number of rows in image part of the detector	1
$N_{\text{column, det}}$	number of columns in image part of the detector	1

24.1.3 Matrix multiplication algorithm: practice

We will now give a practical road map to correct the straylight in the L01b Processor. We use the term *restriction* to denote a conversion of a variable from a fine towards a coarse grid, in this case from an (unbinned) detector grid towards the CKD grid that contains M blocks. Conversely, *prolongation* is the conversion from a coarse towards a fine grid.

Because straylight is not physically restricted to a single band or detector, we will treat all eight bands together, to account for the inter-band straylight, i.e. the straylight in one band caused by the light directly measured in another band. Furthermore, our formalism will take into account the straylight both due to electromagnetic radiation outside the spectral range of all the four spectrometers (out-of-spectral-range straylight) and due to electromagnetic radiation outside the across and along-track field of view (out-of-field straylight). It is to be discussed if measurements or theoretical predictions can give practical information to fill these ‘virtual’ blocks. If it is not possible to obtain this information with sufficient accuracy, the entries in these blocks can be set to zero. The CKD straylight matrix, therefore, is defined for both UVN and SWIR together. Of course, it is likely that the straylight matrix is in fact a block matrix which can be subdivided into smaller parts, related to individual detectors. This may even be necessary for computational reasons since the matrix has to fit into memory. However, this is a mere technical issue.

For the UVN module: For each spectrometer, extract the current image towards an unbinned image. This is done by replicating the rows with binning factor > 1 .

The restriction step: Convert each image defined on the unbinned grid towards the CKD-grid of M_{det} regions. Each unbinned pixel \mathbf{x}_{det} , in each band b , belongs to exactly one region (block) $B[i]$. This information is stored in the mapping $f_{\text{p2b}}[b, \mathbf{x}_{\text{det}}] \rightarrow i, 1 \leq i \leq M_{\text{det}}$. The M_{det} blocks together create a set of blocks \mathbf{B}_{det} . The restriction operator is the average of all pixels signals in the region:

$$S_{\text{block,det}}[i] = \frac{1}{N_{(b, \mathbf{x}_{\text{det}}) \in B[i]}} \sum_{(b, \mathbf{x}_{\text{det}}) \in B[i]} S[\mathbf{x}_{\text{det}}] . \quad (215)$$

An image created by this step is represented as a column vector of length M_{det} .

Remark on binning We can combine these first two steps by immediately using a mapping for the binned image: $f_{\text{p2b}}[b, \mathbf{x}_{\text{img}}] \rightarrow i, 1 \leq i \leq M_{\text{det}}$.

Further, we define the extended image, described by the concatenation of the M_{det} blocks and the M_v virtual blocks, where $M = M_{\text{det}} + M_v$. We acquire the signal in the virtual blocks $\mathbf{S}_{\text{block,virt}}$ with a function $f_{\text{virtual}}[\mathbf{S}_{\text{block,det}}]$ that relates the already computed non-virtual block signals to the virtual block signals. The extended image is given by $\mathbf{S}_{\text{block}} = (\mathbf{S}_{\text{block,det}}^T, \mathbf{S}_{\text{block,virt}}^T)^T$ and consists of $M = M_{\text{det}} + M_v$ values on the CKD-grid.

We now compute the **straylight on the CKD grid** by applying the ‘inner’ part of Equation (212):

$$S_{\text{stray,block}}[i] = [\mathbf{M}_{\text{SL, reduced}} \cdot \mathbf{S}_{\text{block}}][i] . \quad (216)$$

This is the actual matrix multiplication. If, at this stage, only a subset of the straylight block signal is needed (for example, all M_b blocks belonging to a single band b), the corresponding rows in $\mathbf{M}_{\text{SL, reduced}}$ can be chosen, giving a matrix of size $M_b \times M$.

The prolongation step: The straylight signal on the CKD grid is expanded towards all unbinned pixels. Simply broadcasting the same straylight contribution of a block towards all pixels in the block will generate artifacts across the block boundaries. Therefore the prolongation operator involves an additional smoothing or interpolation action, where the following aspects must be taken into account:

- The position of each pixel with respect to block boundaries. This determines which blocks are used in the interpolation.
- A conservation restriction: The total amount of straylight before and after the smoothing must be the same.

We informally write:

$$S_{\text{stray}}[\mathbf{x}_{\text{det}}]_b = f_{\text{prolongation}}[f_{\text{p2b}}^{-1}, S_{\text{stray,block}}] . \quad (217)$$

Note that S_{stray} is defined per band, as per construction of the prolongation operator. The inverse of f_{p2b} does not exist for virtual blocks which is not a problem because we do not have to correct for the straylight in the virtual blocks.

Remarks on the interpolation in the prolongation step. Probably the simplest two-dimensional interpolation procedure that might accomplish sufficient smoothing, is the bilinear interpolation. In this case, it suffices to provide for each detector pixel (\mathbf{x}_{det}) of each band (b) indices of 4 blocks that surround the pixel (indices_{interp} $[\mathbf{x}_{\text{det}}, i]_b$, $i = 1, 2, 3, 4$), and 4 corresponding interpolation coefficients (coeffs_{interp} $[\mathbf{x}_{\text{det}}, i]_b$, $i = 1, 2, 3, 4$). How to determine the interpolation indices and coefficients is described in [RD11]. Once these values are obtained, to calculate the prolonged straylight signal at a detector pixel, we distinguish three different cases.

First, for detector pixels that do not belong to any of the M_{det} blocks, set the corresponding prolonged straylight values to zero:

$$\forall \mathbf{x}_{\text{det}} :: f_{\text{p2b}}[b, \mathbf{x}_{\text{det}}] \notin \mathbf{B}_{\text{det}} \implies S_{\text{stray}}[\mathbf{x}_{\text{det}}]_b = 0 . \quad (218)$$

Second, for detector pixels that are surrounded by 4 blocks, the prolonged straylight signal can be obtained as:

$$S_{\text{stray}}[\mathbf{x}_{\text{det}}]_b = \sum_{i=1}^4 \text{coeffs}_{\text{interp}}[\mathbf{x}_{\text{det}}, i]_b \cdot S_{\text{stray,block}}[\text{indices}_{\text{interp}}[\mathbf{x}_{\text{det}}, i]_b] . \quad (219)$$

Third and final, for detector pixels that are surrounded by less than 4 blocks, use the equation (219) in combination with coeffs_{interp} $[\mathbf{x}_{\text{det}}]_b = (1, 0, 0, 0)$. In other words, there is no interpolation in this case. We might in the future introduce the case of two indices near the edges in order to smooth the straylight signals there.

The next step is the **re-binning of the unbinned straylight image** towards the binned images ; a binned pixel signal is the average of its contributing pixel signals.

Remark on binning We can combine the two previous steps by immediately prolongating the straylight signal towards all binned pixels. The smoothing in spatial direction should take the binning factors into account.

The final step is the **actual straylight correction**:

$$S_o[\mathbf{x}_{\text{img}}]_b = S_i[\mathbf{x}_{\text{img}}]_b - S_{\text{stray}}[\mathbf{x}_{\text{img}}]_b . \quad (220)$$

24.1.4 Error propagation

We identify the following error sources:

- In Equation (209) we multiply the straylight matrix with the measured signal, instead of the direct signal.
- The measurement itself is used for the correction. In particular, the straylight matrix operates on a block signal that contains read-out noise. This is quantified as follows: Define $n_{\text{block},i}$ as the amount of binned pixels in block i . This does not need to be an integer number, since a bin can cross a block boundary. Then

$$\text{Var}_{\text{readout}} S_{\text{block}}[i] = \text{Var}_{\text{readout}} \frac{1}{n_{\text{block},i}} \sum_{j=1}^{n_{\text{block},i}} S[j] = \frac{1}{n_{\text{block},i}^2} \sum_{j=1}^{n_{\text{block},i}} \text{Var}_{\text{readout}} S[j] = \frac{1}{n_{\text{block},i}} \epsilon_{\text{ckd}}^2 . \quad (221)$$

Also, we have to take shot noise into account since we can argue that shot noise only occurs after the optical processes, in forward sense, have been finished.

- The part of the CKD error due to measurement noise.
- The size of the blocks.
- The choice of a direct region given a block.
- The prolongation operator. This operator mostly has a smoothing effect.
- Large gradients due to ghosting.
- The uncertainty in the straylight matrix entries that correspond to the virtual blocks (out-of-field and out-of-spectral-range)

Each entry in the straylight matrix is accompanied by an error term, of which the largest contribution is from calibration measurement noise. Formal error propagation of Equation (216) gives

$$\begin{aligned}
 s_{\text{stray}}^2[i] &= \sum_{j=1}^M M_{\text{SL}}^2[i, j] s_{s, \text{block}}^2[j] + \sum_{j=1}^M s_{M_{\text{SL}}}^2[i, j] S_{\text{block}}^2[j] && \text{(uncorrelated terms)} \\
 &+ 2 \sum_{j=1}^M \sum_{k=j+1}^M M_{\text{SL}}[i, j] M_{\text{SL}}[i, k] s_{s, \text{block}}[j] s_{s, \text{block}}[k] \rho\{S_{\text{block}}[j], S_{\text{block}}[k]\} && \text{(signal correlation)} \\
 &+ 2 \sum_{j=1}^M \sum_{k=j+1}^M s_{M_{\text{SL}}}[i, j] s_{M_{\text{SL}}}[i, k] S_{\text{block}}[j] S_{\text{block}}[k] \rho\{M_{\text{SL}}[i, j], M_{\text{SL}}[i, k]\} && \text{(matrix entries correlation)}
 \end{aligned} \tag{222}$$

Note that we have omitted the terms related to correlations between the straylight matrix and the measured signal: obviously, $\rho\{S_{\text{block}}[j], M_{\text{SL}}[i, k]\}$ are always zero since they are completely independent. We further claim that the third line of the equation also vanishes: $M_{\text{SL}}[i, j]$ has been computed from a different calibration measurement than $M_{\text{SL}}[i, k]$, since the column index of the matrix is related to the stimulus location. We can estimate the error of the signal in a block $s_{s, \text{block}}^2[j]$ as the average over the individual (binned) signals. The error terms $s_{M_{\text{SL}}}^2[i, j]$ are CKD. Nevertheless, the complete evaluation of Equation 222 will be a very hard task.

As discussed, there are many error sources in the straylight correction algorithm. It is very challenging to both take into account all the relevant error sources and estimate very accurately each error and its correlation to other errors. This makes the formal error propagation difficult to implement. Instead, one could try a more pragmatical approach that relies on the straylight calibration measurements. The calibration campaign consists of two types of measurements. One type is used to derive the CKD parameters. The other type is used for verification of both the derived CKD parameters and the straylight correction algorithm. By applying the straylight correction algorithm to the verification measurements, one could estimate the accuracy of the correction algorithm. For example, verification measurements could be made with a broadband white light source that has a limited divergence. Superimposing detector images for different across-track angles, a hole-in-the-cloud scene could be constructed. The residual straylight signal in the hole, after applying the correction algorithm, is a measure of the accuracy of the straylight correction algorithm.

Measuring point spread functions during the calibration measurements offers another possibility for estimating the accuracy of the algorithm. Namely, using the measured point spread functions, an arbitrary Earth scene that has straylight and the measurement noise, could be modeled. Again, the residual straylight signal in the corrected image is a measure of the accuracy of the straylight correction algorithm. Concluding, the evaluation of the error of a signal will be based on calibration measurements instead of formal error propagation.

24.1.5 Alternative: convolution algorithm: concise version

The main ingredient of the convolution algorithm is the convolution between an input signal and a straylight convolution kernel to obtain a straylight signal. In this sense, this algorithm is similar to convolution algorithms used in image processing to sharpen or to smooth images for example. There, images are smoothed or sharpened depending on which convolution kernel is used. In straylight correction, a special straylight convolution kernel is used to calculate the straylight signal for a given input signal.

Because it describes the straylight response of the instrument, the straylight convolution kernel is called the straylight response function. The straylight response function is a CKD parameter, and it is provided as input for the convolution algorithm. Derivation of the straylight response function from on-ground calibration measurements is described in [RD11].

Unlike many other algorithms, the convolution algorithm works per detector, rather than per band. Since the CKDs are delivered per band, this requires merging of the CKDs of the two bands that correspond to a detector. From now on, we will assume that the signals and the parameters of the two bands are merged and we will refer only to the signals and parameters of the detector. In addition, all the operations are assumed to take place on unbinned signals. Hence, if the signals are binned, expand them towards all unbinned pixels.

Let's now picture a detector as being divided into regions, called blocks, where each pixel belongs to a unique block $B[i]$. This definition of blocks is identical to the definition of blocks described in Section 24.1.3, with the exception that the block map of the convolution algorithm is not unique for all the four detectors, but only for a single detector. A block map which contains the information on how each pixel maps to a unique block of a detector is a CKD parameter, and therefore will be used as input for the convolution algorithm. Derivation of the block map from on-ground calibration measurements is described in [RD11].

For a detector divided in M_{det} blocks, we can write the input detector signal \mathbf{S}_i as a superposition of detector signals $\mathbf{S}_{\text{block}}[i]$:

$$\mathbf{S}_i[\mathbf{x}_{\text{det}}] = \sum_{i=1}^{M_{\text{det}}} \mathbf{S}_{\text{block}}[i][\mathbf{x}_{\text{det}}] , \quad (223)$$

where

$$\mathbf{S}_{\text{block}}[i][\mathbf{x}_{\text{det}}] = \begin{cases} \mathbf{S}_i[\mathbf{x}_{\text{det}}] & \text{for } \mathbf{x}_{\text{det}} \in \mathbf{B}[i] , \\ 0 & \text{for } \mathbf{x}_{\text{det}} \notin \mathbf{B}[i] . \end{cases} \quad (224)$$

Dividing a detector in blocks is done for a purpose. Namely, a unique instrument response function $\mathbf{S}_{\text{insrf}}[i]$ and straylight response function $\mathbf{S}_{\text{srf}}[i]$, can be assigned to each block. Here, the instrument response function is the response of the instrument that is characterized by the instrument spectral response function (ISRF) and pixel response function (PRF). Equation 223 can then be written as follows:

$$\mathbf{S}_i = \sum_{i=1}^{M_{\text{det}}} \mathbf{S}_{\text{block,true}}[i] \otimes (\mathbf{S}_{\text{insrf}}[i] + \mathbf{S}_{\text{srf}}[i]) , \quad (225)$$

where \otimes is the convolution operator, and $\mathbf{S}_{\text{block,true}}[i]$ is the true signal being measured by the instrument as $\mathbf{S}_{\text{block}}[i]$. The signal corrected for straylight, \mathbf{S}_o , can be obtained as:

$$\mathbf{S}_o = \mathbf{S}_i - \mathbf{S}_{\text{stray}} , \quad (226)$$

where

$$\mathbf{S}_{\text{stray}} = \sum_{i=1}^{M_{\text{det}}} \mathbf{S}_{\text{block,true}}[i] \otimes \mathbf{S}_{\text{srf}}[i] . \quad (227)$$

Strictly speaking, the straylight signal, $\mathbf{S}_{\text{stray}}$, can be calculated from Equation 227 only if the true signal value is known. However, for a system with low straylight, the following approximation can be made:

$$\mathbf{S}_{\text{stray}} \approx \sum_{i=1}^{M_{\text{det}}} \mathbf{S}_{\text{block}}[i] \otimes \mathbf{S}_{\text{srf}}[i] , \quad (228)$$

making it possible to calculate the straylight signal from signals $\mathbf{S}_{\text{block}}[i]$, which are measured by the instrument.

Theoretical background We will elaborate on the convolution and the approximation in a more strict mathematical way. Since convolution is a linear operator, we can rewrite the straylight signal (227) (restricting ourselves to one block for the moment) as a matrix operation:

$$\mathbf{S}_{\text{stray}} = \mathbf{R}\mathbf{S}_o \quad (229)$$

Here we associate \mathbf{S}_o with the true signal (the signal after straylight correction) and both \mathbf{S}_i and \mathbf{S}_o are written as vectors: the whole image is reshaped (in reading order, for example) as a 1D-vector.

Note that this is a similar writing as used in the matrix method with block sizes of 1x1 pixel: see, for example, Equation (206). Therefore, the matrix method and the convolution method are strongly related.

The square straylight matrix \mathbf{R} (of size $n_{\text{pix}} \times n_{\text{pix}}$) has zeros on the diagonal. On each row associated with an interior pixel (strictly speaking, a pixel that is farther than half the convolution kernel size away from the boundary), all kernel elements are present somewhere while all other entries in that row are zeros. Note that a convolution will in practice never be computed using this matrix notation: not only is the matrix dimension simply too large for that; much faster convolution implementations exist (see below).

Now, we can proceed using Equation (226) and write $\mathbf{S}_o = \mathbf{S}_i - \mathbf{R}\mathbf{S}_o$ or $(\mathbf{I} + \mathbf{R})\mathbf{S}_o = \mathbf{S}_i$. However, if we want the straylight correction to preserve ‘mass’, i.e. if we do not want that the total amount of signal on the detector decreases, we can introduce the concept of *kernel energy* U : the sum of all convolution kernel entries, being the same as the sum of one row of \mathbf{R} . The straylight subtraction then becomes a subtraction-with-scaling:

$$((1 - U)\mathbf{I} + \mathbf{R})\mathbf{S}_o = \mathbf{S}_i \quad (230)$$

Because of the absolute radiometric correction algorithm steps, conservation of signal is not important; therefore, for UVN at least, we set $U = 0$.

We want to solve the linear system (230): the right-hand side is the measured signal, while the unknown variable is the straylight-corrected signal. We apply Jacobi iterations:

$$\mathbf{S}_o^{m+1} = \mathbf{D}^{-1} [\mathbf{S}_i - \mathbf{R}\mathbf{S}_o^m] \quad (231)$$

where $\mathbf{D} = (1 - U)\mathbf{I}$, the diagonal of the matrix. For the initial estimate we set $\mathbf{S}_o^0 = \mathbf{S}_i$. The Jacobi method converges if the matrix is diagonally dominant, thus for $U < 0.5$. The first Jacobi iteration gives

$$\mathbf{S}_o^1 = \mathbf{D}^{-1} [\mathbf{S}_i - \mathbf{R}\mathbf{S}_i] = \frac{1}{1-U} (\mathbf{I} - \mathbf{R})\mathbf{S}_i \quad (232)$$

For $U = 0$, this gives as correction:

$$\mathbf{S}_o^1 = \mathbf{S}_i - \mathbf{R}\mathbf{S}_i. \quad (233)$$

The approximation mentioned above is therefore the result of one Jacobi-iteration. This ends the part on the mathematical background.

The convolution operation can be written as a double sum:

$$S_{\text{stray}}[r_{\text{det}}, c_{\text{det}}] = \sum_{i=1}^{M_{\text{det}}} \sum_{w=-\frac{W-1}{2}}^{\frac{W-1}{2}} \sum_{v=-\frac{V-1}{2}}^{\frac{V-1}{2}} S_{\text{block}}[i][r_{\text{det}} - w, c_{\text{det}} - v] \cdot S_{\text{slrf}}[i][w, v]. \quad (234)$$

The two iterating parameters w and v of $S_{\text{slrf}}[i]$ are denoted differently from the two iterating parameters r_{det} and c_{det} for a reason. While iterator parameters r_{det} and c_{det} can take on values $0, 1, \dots, N_{\text{row,det}} - 1$ and $0, 1, \dots, N_{\text{column,det}} - 1$ respectively, iterator parameters w and v can take on values $-\frac{W-1}{2}, -\frac{W-1}{2} + 1, \dots, \frac{W-1}{2}$ and $-\frac{V-1}{2}, -\frac{V-1}{2} + 1, \dots, \frac{V-1}{2}$ respectively. Here, $N_{\text{row,det}} - 1, N_{\text{column,det}} - 1, \frac{W-1}{2}$, and $\frac{V-1}{2}$ are positive integers (See Table 24.1.2 for a description of parameters $N_{\text{row,det}}, N_{\text{column,det}}, W$, and V). As a consequence, the two indices of $S_{\text{slrf}}[i]$, w and v , can be negative. In contrast, this is not the case for the two indices r_{det} and c_{det} .

Note that $S_{\text{block}}[i][r_{\text{det}} - w, c_{\text{det}} - v]$ is not defined for cases where at least one of the two parameters $r_{\text{det}} - w$ and $c_{\text{det}} - v$ is negative. In those cases one could for example impose $S_{\text{block}}[i][r_{\text{det}} - w, c_{\text{det}} - v] = 0$. This solution is attractive if the dimensions of the convolution kernel are not large. If this approach introduces significant additional features in the corrected images, it would be prudent to consider extending S_{block} by means of extrapolation to obtain valid values for all the terms in the double sum.

The larger the dimensions of the convolution kernel, the more computationally intensive is to calculate the double sum. If this operation impedes the performance of the I01b processor, it is advised to consider an implementation of the convolution operation that makes use of the fast Fourier transform (FFT). According to the convolution theorem, the Fourier transform of the convolution of two functions is equal to the product of their individual Fourier transforms. Therefore, it might be computationally more favorable to perform a fast Fourier transform on the two functions, multiply their individual Fourier transforms, and then perform the inverse FFT on the product, rather than to calculate the double sum.

Another way to further improve the performance of the I01b processor, would be to use a mean straylight response function for each detector, and hence compute only one convolution per detector. In this case, it is not necessary to derive a block map for each detector, because each detector consists of only one block. If the differences between individual straylight response functions are not large, the mean straylight response function approach might give results with acceptable accuracy.

Once S_{stray} is calculated, the output signal S_o is obtained in a subtraction step, similar to the matrix multiplication algorithm:

$$S_o[\mathbf{x}_{\text{img}}]_b = S_i[\mathbf{x}_{\text{img}}]_b - S_{\text{stray}}[\mathbf{x}_{\text{img}}]_b, \quad (235)$$

where the straylight signal has of course been binned according to the current binning scheme.

24.1.6 SWIR straylight

In the SWIR detector, straylight is modeled the same way using the convolution principle. The correction algorithm is, however, different in three aspects:

- **Iterative approach** The total straylight fraction is estimated to be 6.7%. This makes the approximation in Equation (233) less accurate. Therefore, *three* Jacobi iterations of (230) are used.
- **Energy conservation** The energy is chosen as the sum of the kernel elements: $U = 0.067$.

- **Additional reflection kernel** Straylight in the form of a spatial reflection is modeled using an additional convolution kernel \mathbf{M} . Taken together, the straylight correction is the result of four consecutive convolutions:

$$\mathbf{S}_{\text{stray}} = \mathbf{S}_i - (\mathbf{S}_0^3 - \mathbf{M}\mathbf{S}_0^3) \quad (236)$$

24.1.7 Out-of-band straylight correction for the NIR detector

This correction step is performed before the regular straylight correction. It is applicable for the NIR detector only. The correction is performed twice: first for straylight for wavelengths higher than the NIR detector wavelength range ('red'), then for wavelengths smaller than the detector wavelength range ('blue'). The L01b Algorithm is only applicable for measurements in specific processing classes: (special) radiance and (special) irradiance. Per processing class, a CKD is defined that consists of eleven images, each image is based on the straylight response stemming from row illumination via a fibre transmitting a laser signal in the on-ground calibration. The algorithm basically combines these eleven images based on the magnitude of an in-band reference signal (i.e. measured by the NIR-detector itself) at each row. The CKD images, in turn, are a superposition of raw laser measurements: a weighted average where the weights are determined by the expected spectral behaviour of the light source (Sun, radiance or calibrated lamp) at the out-of-spectral-band wavelengths.

Parameter	Description	Units
$S_{\text{oob}}[f][\mathbf{x}_{\text{det}}]$	Normalized out-of-band signal for fibre f	1
λ_{m^*}	Characteristic in-band wavelength	nm
$S(\lambda_{m^*})$	Characteristic actual in-band signal	$\text{e}^{-\text{s}^{-1}\text{nm}^{-1}}$
$S_{\text{total,oob}}[\mathbf{x}_{\text{det}}]$	Constructed image containing all out-of-band straylight	$\text{e}^{-\text{s}^{-1}}$

The input, for both 'red' and 'blue':

- The barycentre of the fibres, together with the virtual barycentre of two extended fibres, expressed in detector rows $r_{f,p}$, $p = 0, 12$. This is a CKD attribute.
- The anchor in-band wavelength λ_{m^*} , given as a configuration parameter.
- The eleven images $S_{\text{total,oob}}[f][\mathbf{x}_{\text{det}}]$.
- A non-linear function H , given as a look-up table configuration parameter. This function is a refinement over the relative spectral density table.

Step 1. Defining the anchor in-band signal. For each measurement, the representative in-band signal $S(\lambda_{m^*})$, for all image rows, has to be determined. This signal is expressed *per nanometer*.

$$S_{\text{ib}}[r_{\text{img}}] = \frac{n_{\text{cols-per-nm}}}{n_{\text{cols}}} \sum_{c \in \text{cols}} S[r_{\text{img}}, c] \quad (237)$$

In the initialization phase, the wavelength map can be used to determine the pixels associated with wavelength λ_{m^*} , and the width, in nm, of one pixel. The in-band signal can for example be constructed as the summed signal of *ca.* seven adjacent pixels in a row. Alternatively, the pixel closest to λ_{m^*} can be used together with a division by the pixel width (in nm).

Step 2. Construct the total out-of-band image. The next step is interpolation in row direction to assemble a total out-of-band image. This image is a linear combination of the 11 out-of-band images per fibre. We start with defining the out-of-band image for an arbitrary row between two 'fibre rows' $r_{f,p}$ and $r_{f,p+1}$:

$$S_{\text{total,oob}}[r][\mathbf{x}_{\text{det}}] = S_{\text{ib}}[r] \frac{1}{r_{f,p+1} - r_{f,p}} [(r_{f,p+1} - r)S_{\text{oob}}[f_p][\mathbf{x}_{\text{det}}] + (r - r_{f,p})S_{\text{oob}}[f_{p+1}][\mathbf{x}_{\text{det}}]]. \quad (238)$$

In the end, the total out-of-band straylight image is simply a linear combination of the eleven $S_{\text{oob}}[f][\mathbf{x}_{\text{det}}]$:

$$S_{\text{total,oob}}[\mathbf{x}_{\text{det}}] = \sum_{p=1}^{11} D_p S_{\text{oob}}[f_p][\mathbf{x}_{\text{det}}], \quad (239)$$

where

$$D_p = \left(\sum_{r=r_{f,p-1}+1}^{r_{f,p}} \frac{r - r_{f,p-1}}{r_{f,p} - r_{f,p-1}} S_{ib}[r] \right) + \left(\sum_{r=r_{f,p+1}}^{r_{f,p+1}-1} \frac{r_{f,p+1} - r}{r_{f,p+1} - r_{f,p}} S_{ib}[r] \right). \quad (240)$$

This equation implies detector rows and unbinned signals. Further, in D_p neighbouring indices $p - 1$ and $p + 1$ are used. That implies that we need two ‘boundary case’ images: We may assume the boundary fibres f_0 and f_{12} and corresponding out-of-band straylight images: $S_{oob}[f_0] = S_{oob}[f_1]$ and $S_{oob}[f_{12}] = S_{oob}[f_{11}]$ with associated row barycentres for these virtual fibres. Therefore, Equation 239 needs to be extended with the terms for $p = 0$ and $p = 12$, while the associated D_0 and D_{12} consist of only one term instead of two.

In this step, we can immediately switch to binned images using the binning table associated with the measurement. This gives $S_{total,oob}[\mathbf{x}_{img}]$ where the $S_{ib}[r]$ needed in D_p is simply a sequence of replications of $S_{ib}[r_{img}]$.

Extension of D_p :

Instead of using Equation 240, we introduce an extra relationship:

$$D_p = \left(\sum_{r=r_{f,p-1}+1}^{r_{f,p}} \frac{r - r_{f,p-1}}{r_{f,p} - r_{f,p-1}} H(S_{ib}[r]) \right) + \left(\sum_{r=r_{f,p+1}}^{r_{f,p+1}-1} \frac{r_{f,p+1} - r}{r_{f,p+1} - r_{f,p-1}} H(S_{ib}[r]) \right) \quad (241)$$

Here the function H serves as an addendum to the imposed spectral density to allow more flexibility in the correction. The default situation is the identity operation: $H(S) = S$. Adjustments can be made according to in-orbit analysis results.

Step 3. Correct the image for out-of-band straylight. The final step is the actual subtraction:

$$S_o[\mathbf{x}_{img}] = S_i[\mathbf{x}_{img}] - S_{total,oob}[\mathbf{x}_{img}]. \quad (242)$$

As noted above, the error will not be formally propagated but will be assessed after analysis of in-flight measurements.

24.2 Slit irregularity correction

The manufacturing process of the slit is not perfect; that means that the slit width is not constant. Therefore a viewing angle dependence is expected to be present. This irregularity can be expressed in the slit irregularity function $f_{slit}[r_{det}]$, wherein a row dependency is expressed. Note that smile effects are already incorporated.

The retrieval of the slit irregularity from a WLS measurement includes a summing/averaging step in the spectral direction. By doing so, PRNU effects are removed, and a row-dependent response curve remains that includes both low-spatial-frequency variations and high-spatial-frequency variations. The latter variations are assigned to slit irregularity. Note that we hereby *define* the slit irregularity as the high-frequency row-to-row variation, where the average over all columns in each row is considered. That means that features that might exist in reality, like a spatial smile or a slight overall rotation of the slit with respect of the along-track direction, are not accurately described using this definition. However, this is not a major problem since these features are corrected by other algorithms like PRNU and radiance/irradiance. It is probably best to describe the slit irregularity correction as the correction of the *projection* of the slit irregularity on the row direction.

24.2.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} before correction	$e^- s^{-1}$
$\sigma_i^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$e^{-2} s^{-2}$
$S_o[\mathbf{x}_{img}]$	signal in image pixel \mathbf{x}_{img} after correction	$e^- s^{-1}$
$\sigma_o^2[\mathbf{x}_{img}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$e^{-2} s^{-2}$
$f_{slit}[r_{det}]$	slit irregularity factor	none

24.2.2 Algorithm description

Like the PRNU correction, the slit irregularity is expressed as a factor:

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] \frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{slit}}[r_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} . \quad (243)$$

24.2.3 Error propagation

The error caused by the slit irregularity correction is propagated directly using the product rule of the formal error propagation mechanism:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \left(\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{slit}}[r_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + \overline{s_{f_{\text{slit}}}^2[r_{\text{det}}]} S_i[\mathbf{x}_{\text{img}}]^2 . \quad (244)$$

Note that the variance of the slit irregularity function f_{slit} can depend on the row number. We make again use of the definition of the mean unbinned variance described in Section 20.4.2.

24.3 Flat fielding

This correction is for the internal stimuli (LED, WLS) and *not* part of the direct correction of (ir)radiance. The calibration key data is derived from the unbinned image response of an illumination by LED or WLS. Subsequent measurements by internal stimuli are normalized by the calibrated image fields. This results in a uniform field with values close to unity. In this way, in-flight degradation of the different elements of the instrument can be monitored.

24.3.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$e^- s^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$e^{-2} s^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	1
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	1
$S_{\text{ckd}}[\mathbf{x}_{\text{det}}]$	reference CKD signal	$e^- s^{-1}$
$s_{\text{ckd}}^2[\mathbf{x}_{\text{det}}]$	variance of reference CKD signal	$e^{-2} s^{-2}$

24.3.2 Algorithm description

The flat fielding per pixel is described as the following factor:

$$c_{\text{flat}}[\mathbf{x}_{\text{img}}] = 1/\overline{S_{\text{ckd}}[\mathbf{x}_{\text{img}}]} . \quad (245)$$

Here,

$$\overline{S_{\text{ckd}}[\mathbf{x}_{\text{img}}]} = (1/N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}) \sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} S_{\text{ckd}}[\mathbf{x}_{\text{det}}] \quad (246)$$

is the averaged reference stimulus field obtained during the calibration. The correction is now expressed as:

$$S_o[\mathbf{x}_{\text{img}}] = c_{\text{flat}}[\mathbf{x}_{\text{img}}] S_i[\mathbf{x}_{\text{img}}] . \quad (247)$$

24.3.3 Error propagation

We define the mean inverted variance as

$$\overline{s_{\text{flat}}^2[\mathbf{x}_{\text{img}}]} = \frac{1}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \frac{1}{s_{\text{ckd}}^2[\mathbf{x}_{\text{det}}]} , \quad (248)$$

so that the error propagation can be expressed as:

$$\sigma_0^2[\mathbf{x}_{\text{img}}] = c_{\text{flat}}^2[\mathbf{x}_{\text{img}}] \sigma_i^2[\mathbf{x}_{\text{img}}] + \overline{s_{\text{flat}}^2[\mathbf{x}_{\text{img}}]} S_i[\mathbf{x}_{\text{img}}]^2 . \quad (249)$$

Note that the error in the flat field correction is propagated directly using the product rule of the formal error propagation mechanism. The usual caveats with respect to binning (see Section 20.4.2) hold. Further, we should be aware of the fact that the variance appears in the denominator. From theory on stochastic division, it is known that a bias will be introduced. This bias, which is a function of the ratio between mean signal and standard deviation in the denominator, is probably very small. Once the CKD is known, we can decide if it is necessary to correct for this additional bias.

24.4 On irradiance, radiance and BSDF

In the following sections, 24.5 through 24.9, the correction algorithms that transform light fluxes (measured in electrons per second) towards radiance and irradiance (measured in $\text{mols}^{-1}\text{m}^{-2}\text{nm}^{-1}$ and $\text{mols}^{-1}\text{m}^{-2}\text{nm}^{-1}\text{sr}^{-1}$, respectively) are described. The radiance and irradiance are connected via the TROPOMI instrument bidirectional scattering distribution function (BSDF).

For several reasons, including limitations following from measurement possibilities, the calibration measurements ultimately provide two CKDs for both radiance and irradiance, and a BSDF factor CKD. These are:

Irradiance: $f_{\text{absirr}}[\mathbf{x}_{\text{det}}]$ and $f_{\text{relirr}}[\mathbf{x}_{\text{det}}, \phi, \varepsilon]$. The absolute conversion factor f_{absirr} describes the relation between the flux and irradiance for nominal Sun angles. The underlying measurements are performed with a calibrated light source. Thereafter, a dimensionless correction factor f_{relirr} describes the dependencies with non-nominal Sun angles. Here the underlying measurements are performed with an uncalibrated, albeit stable, light source. Hence the division between the two CKDs, each accompanied by their own error.

Radiance: $f_{\text{absrad}}[\mathbf{x}_{\text{det}}]$ and $f_{\text{relrad}}[\mathbf{x}_{\text{det}}]$. The absolute conversion factor f_{absrad} describes the relation between the flux and radiance. Again, a calibrated light source is used. Moreover, the measurements are only performed for a limited number of (central) rows. For other rows, the f_{absrad} CKD is duplicated along spectral lines. The radiance measurements for the other, non-central rows are performed with an uncalibrated light source and anchored to the absolute central row measurements, giving the relative correction f_{relrad} . These measurement setups again naturally lead to two different CKDs with their own error.

BSDF: $f_{\text{bsdf}}[\mathbf{x}_{\text{det}}]$. Per definition, $f_{\text{bsdf}} = \frac{f_{\text{absrad}}}{f_{\text{absirr}}}$. (Note that the instruments BSDF equals irradiance response divided by radiance response, but in the inverse model, with multiplicative f 's, we need the reciprocal expression!) However, the BSDF function can also be derived with an uncalibrated stable light source that performs measurements through the instrument's Sun port and Earth port. Hereto quantities like vacuum chamber window transmittances, distances between light source and diffusers, and the BSDF of the external diffuser in the Earth port measurement are needed. Without going into these calibration details, we can assume that the BSDF CKD can thus be acquired using this alternative approach.

The triangular relation between radiance, irradiance and instrument BSDF enables us to choose the most optimal route to derive one of the three CKDs using two CKDs with the smallest error involved. This decision can alter once more data is available. Without loss of generality, we can assume that the absolute and relative radiance and irradiance are available as CKD and they will be used in the sections that follow.

This approach holds for both UVN and SWIR detectors.

24.5 Irradiance responsivity

The irradiance responsivity correction implements the relation between the charge (measured in electrons) as generated in the detector and the absolute photon irradiance (measured in $\text{mols}^{-1}\text{m}^{-2}\text{nm}^{-1}$) at the nominal Sun azimuth and elevation angles. For Sun positions other than the nominal one (zero azimuth and elevation), an additional correction is needed; this is described in Section 24.6. This algorithm step is only needed for the Solar_irradiance processing class.

24.5.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$e^- s^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$e^{-2} s^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	$\text{mol m}^{-2} \text{nm}^{-1} \text{s}^{-1}$
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} \text{s}^{-2}$
$f_{\text{absirr},d}[\mathbf{x}_{\text{det}}]$	conversion factor, depending on diffuser d	$\text{mol m}^{-2} \text{nm}^{-1} (e^-)^{-1}$
$s_{f,\text{absirr},d}^2[\mathbf{x}_{\text{det}}]$	variance of conversion factor	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} (e^-)^{-2}$

24.5.2 Algorithm description

$$S_o[\mathbf{x}_{\text{img}}] = \frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{absirr},d}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} S_i[\mathbf{x}_{\text{img}}] . \quad (250)$$

The on-ground calibration provides the calibration key data $f_{\text{absirr},d}[\mathbf{x}_{\text{det}}]$.

24.5.3 Error propagation

The on-ground calibration provides the calibration key data $s_{f,\text{absirr},d}^2[\mathbf{x}_{\text{det}}]$. if we can assume that the variance is independent of rows and columns, then:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \left(\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{absirr},d}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + \frac{S_i[\mathbf{x}_{\text{img}}]^2}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}^2} \sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} s_{f,\text{absirr},d}^2[\mathbf{x}_{\text{det}}] . \quad (251)$$

Here the N^2 in denominator follows from the averaging of the unbinned CKD. However, it is safer to assume at least some correlations. In that case, and up to cases of perfect correlation, we have an upper estimate:

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \left(\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{absirr},d}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + S_i[\mathbf{x}_{\text{img}}]^2 \overline{s_{f,\text{absirr},d}^2[\mathbf{x}_{\text{det}}]} . \quad (252)$$

Note that we have used the mean variance $\overline{s_{f,\text{absirr},d}^2[\mathbf{x}_{\text{det}}]}$ to indicate that the variances of the unbinned signals can all be substituted with a single binned signal variance. This has been discussed in Section 20.4.2.

24.6 Relative irradiance responsivity

The irradiances as computed using the irradiance responsivity correction (Section 24.5) pertain to the Sun azimuth and elevation angles at the time of the measurement. The relative irradiance algorithm translates these irradiances to irradiances at the nominal Sun azimuth and elevation angles. This algorithm step is only needed for the Solar_irradiance processing class.

24.6.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$\text{mol m}^{-2} \text{nm}^{-1} \text{s}^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} \text{s}^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	$\text{mol m}^{-2} \text{nm}^{-1} \text{s}^{-1}$
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} \text{s}^{-2}$
$f_{\text{relirr},d}[\mathbf{x}_{\text{det}}, \varphi, \varepsilon]$	correction factor, depending on diffuser d	1
$s_{f,\text{relirr},d}^2[\mathbf{x}_{\text{det}}, \varphi, \varepsilon]$	variance of correction factor	1
φ	Sun azimuth angle	rad
ε	Sun elevation angle	rad

24.6.2 Algorithm description

From the on-ground calibration, a CKD parameter f_{relirr} is provided that describes the dependence on Sun azimuth angle φ and elevation angle ε . The primary information source are the irradiances measured on grid points of a grid consisting of n_{azimuth} by $n_{\text{elevation}}$ grid nodes. For angles in between, some kind of interpolation is used. Using this interpolation, we can define the four-dimensional Sun angle dependence function as

$$f_{\text{relirr},d}[\mathbf{x}_{\text{det}}, \varphi, \varepsilon] : \mathbb{N}^2 \times \mathbb{R}^2 \rightarrow \mathbb{R}, \quad (253)$$

where φ and ε are acquired from geometrical annotation. The irradiances are then converted as

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] \frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{relirr},d}[\mathbf{x}_{\text{det}}, \varphi, \varepsilon]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}}. \quad (254)$$

We have to stress that the on-ground CKD $f_{\text{relirr},d}$ is based on a very coarse grid in the azimuth and elevation dimensions. After launch, much more in-flight calibration measurements will be performed in these angular dimensions. That poses an interesting question how to adjust (or re-define) the in-flight CKD $f_{\text{relirr},d}$. We mention:

- The measurements in the angular dimensions will be locally dense. This makes it difficult to specify a table-like data structure (hypercube) without running into memory problems.
- Consequently, a derived smooth function from these irregularly spaced measurements will have varying levels of accuracy.
- Measurements of different timestamps have to be weighted in a certain way before fitting a function for f_{relirr} . More specific, when do we have to discard older measurements? This question is related to degradation issues.
- The relation with the absolute radiance f_{absrad} , defined as on-ground CKD, has to be taken into account. Again, degradation will play a role here.

In all cases, the CKD f_{relirr} must be defined for each pixel \mathbf{x}_{det} and all values of φ and ε inside sufficiently large intervals. Just keeping the information from calibration measurements in tabulated form is hardly doable for the on-ground measurements (given, say, ten angles in each direction, the CKD would contain 50 million values per band). The in-flight measurements provide some orders of magnitude more data. Clearly, the CKD has to be parametrized in some dimensions. The questions now arise exactly which dimensions have to be parametrized and what kind of parametrization must be used.

Available data and smoothness On the one hand, we will have measurements available for all pixels (for on-ground calibration, this means unbinned pixels; in-flight, the measurements may consist of binned images). On the other hand, the two-dimensional angular grid will in all cases be covered with a grid of certain sparseness. This angular grid gives a clue of the unknown actual smoothness in the two angular directions, while for each chosen angle combination the smoothness along rows and columns can directly be assessed.

What kind of parametrization must be used? The precision of a measurement in the four-dimensional space determines the parametrization choice. If the error (this includes the noise, since f_{relirr} is a CKD) is very small, then any polynomial fit that intends to describe the relative radiance in one or more dimensions will have a lack of fit in the measurement points themselves, not to mention the error that is raised by the finite order of the polynomial. Here we assume that the polynomial order in a direction is lower than the number of measurement points.

An alternative is to define a spline in one direction that passes exactly through the measured points. A cubic spline involves $4n$ coefficients for n measurement points – that is quite a lot. If, however, we perform the spline computation not as part of the calibration algorithm but in the L01b Processor itself (using a tabulated CKD) we save this factor of four.

Reduction in number of pixels Given a certain parametrization of the angle dependencies for each pixel, the size of the potential CKD will be near its upper limit. If the angular surface does not vary much from pixel to pixel, a reduction can be attained by defining a grid of pixels (in row or column direction, or both). For example, we can choose to administrate the angular surface description only for binned rows, and with a

certain stride between columns. Note that the pixel grid size need not to be constant and can be locally decreased (even up to the old minimum of one pixel distance) when necessary. When $f_{\text{relirr}}[\mathbf{x}_{\text{img}}, \varphi, \varepsilon]$ is needed, we can collect the four surrounding ‘corners’ $f_{\text{relirr}}[\mathbf{x}_{\text{ll}}, \varphi, \varepsilon]$, $f_{\text{relirr}}[\mathbf{x}_{\text{lr}}, \varphi, \varepsilon]$, $f_{\text{relirr}}[\mathbf{x}_{\text{rl}}, \varphi, \varepsilon]$ and $f_{\text{relirr}}[\mathbf{x}_{\text{rr}}, \varphi, \varepsilon]$ and use bilinear or bicubic interpolation in the L01b Processor to give the approximation $\tilde{f}_{\text{relirr}}[\mathbf{x}_{\text{img}}, \varphi, \varepsilon]$. This is only sensible, however, if the maximum error is small enough for all measured angles: $\| \tilde{f}_{\text{relirr}}[\mathbf{x}_{\text{img}}, \varphi, \varepsilon] - f_{\text{relirr}}[\mathbf{x}_{\text{img}}, \varphi, \varepsilon] \| \leq \delta, \forall \varphi, \forall \varepsilon$. A related option is to define the coarse grid for row and wavelength and use a similar interpolation as above, but now based on the associated wavelength of \mathbf{x}_{img} .

An alternative of administrating the relative irradiance per pixel or on a pixel grid as described here, is to perform a complete parametrization in row direction or column direction. Also, after a transformation to a wavelength grid, a parametrization in wavelength direction instead of column direction might be an option.

Numerical issues of parametrizations We now elaborate on problems involved in the parametrization of the relative irradiance in certain dimensions. Spline interpolation in one dimension is rather robust, once outliers in measurements (due to low signal-to-noise ratios) can be guaranteed to be absent. Two-dimensional splines, for example for describing the two angular dimensions simultaneously, are well doable (although cumbersome when performed in the L01b Processor) for splines of order 3 (order 1 boils down to bilinear interpolation), but higher orders are not recommended (and probably not necessary anyway) due to the high-order derivatives involved.

If we want to parametrize one or more dimensions using polynomials, numerical stability demands that the domain must be normalized. Moreover, a fit using higher polynomial orders is dangerous if ordinary polynomials serve as base functions; therefore Chebyshev polynomials are a better option (see Appendix A).

One technique is to find a polynomial description for one direction first (say, the elevation) for each three-dimensional grid point (here: per pixel, for all azimuth grid measurements):

$f_{\text{relirr}}[\mathbf{x}_{\text{img}}, \varphi_i](\varepsilon) = \sum_{j=0}^{N_\varepsilon} c_j[\mathbf{x}_{\text{img}}, \varphi_i] T_j(\tilde{\varepsilon})$. One can then try to fit a polynomial through each polynomial coefficient in the second dimension (say, the azimuth):

$$c_j[\mathbf{x}_{\text{img}}](\varphi) = \sum_{k=0}^{N_\varphi} d_k[\mathbf{x}_{\text{img}}] T_k(\tilde{\varphi}), \quad 0 \leq j \leq N_\varepsilon. \quad (255)$$

However, in this way the correlation between each of the coefficients c_j is not taken into account. That is, each of the coefficients is fitted separately while the original cost function (the deviation from f_{relirr}) is not directly taken into account.

A potentially better approach would be to fit the two-dimensional polynomial expression $\sum \sum d_{jk} T_j(\tilde{\varepsilon}) T_k(\tilde{\varphi})$ directly. We call this the simultaneous two-dimensional fit, in contrast to the sequential two-dimensional fit described above. A potential drawback here is that the polynomial matrix $A_{jk} = T_j(\varepsilon_j) T_k(\varphi_k)$ can have a high condition number (compared to the polynomial matrices of the two sequential one-dimensional polynomial fits, where the characteristics of the orthogonal Chebyshev polynomials ensure very low condition numbers). High condition numbers in linear systems can cause severe numerical problems.

A third alternative for a polynomial fit is to write the approximation as $(\sum T_j(\tilde{\varepsilon})) \cdot (\sum T_k(\tilde{\varphi}))$. In this case, a formal separation of the two angular variables is imposed. The fit for each variable uses the deviation from the averaged (along the other variable) f_{relirr} as cost function. The great advantage of this method is that only $N_\varepsilon + N_\varphi$ coefficients need to be fitted, instead of $N_\varepsilon \cdot N_\varphi$ coefficients in the two-dimensional polynomial fit. However, we do not know beforehand whether the actual evaluation of the fit does not result in large deviations.

After addressing the questions above, we state the baseline approach to be the following:

- We first establish a pixel stride in both row and column directions. These strides do not need to be constant. This gives a coarse pixel grid $(\mathbf{r}_{\text{img,coarse}}, \mathbf{c}_{\text{img,coarse}})$. Global grid refinement is possible. In the extreme case, the coarse grid is equal to the normal detector grid. The pixel stride must be chosen such that the error resulting from bilinear/bicubic interpolation in the L01b Processor, computed for each image pixel, is below a certain threshold.

A slight extension is to make the grid curved: $(\mathbf{r}_{\text{img,coarse}}, \mathbf{c}(\mathbf{r}))$. This supports a wavelength grid: the vertical curves are wavelength-isolines. Interpolation proceeds similarly as above (assuming that the curves run parallel, the ‘horizontal’ weighting factors are uniquely defined).

- Then, per pixel in the coarse image grid, a two-dimensional polynomial fit is performed using one of the three fit approaches explained above, where the baseline is the simultaneous two-dimensional polynomial fit. See the Appendix for details on two-dimensional Chebyshev polynomials.

We stress that this baseline approach will be reassessed once new data (on-ground and in-flight) is available. Note that, when a new in-flight measurement (with a new angular configuration) becomes available, this measurement will be stored when its quality is judged satisfactory. A new two-dimensional polynomial fit can then be performed, resulting in an adjusted CKD.

Ultimately, a compromise $f_{\text{relirr},d}$ CKD with a minimal overall error per pixel, based on the allowed size of the CKD, the measurement error and the parametrization, has to be found.

24.6.3 Error propagation

On-ground calibration provides the error $s_{f_{\text{relirr},d}}^2[\mathbf{x}_{\text{det}}, \varphi, \varepsilon]$. If evaluated for a certain angle combination (according to the baseline, see above), we have as a processed CKD error $s_{f_{\text{relirr},d}}^2[\mathbf{x}_{\text{det}}]$. We do not need information about the smoothness of the variance function in the two angular directions. Because of the binning operation, knowledge about the correlations between individual uncorrelated Sun angles in the row direction is needed. For now, we assume the correlations are perfect, hence

$$\sigma_0^2[\mathbf{x}_{\text{img}}] = \left(\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{relirr},d}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + S_i[\mathbf{x}_{\text{img}}]^2 \overline{s_{f_{\text{relirr},d}}^2[\mathbf{x}_{\text{det}}, \varphi, \varepsilon]} . \quad (256)$$

Here we again make use of the definition of the mean unbinned variance described in Section 20.4.2.

24.7 Irradiance averaging

The diffusers can introduce random-like features in the measured Sun spectrum. These features show up in the Sun-normalised radiance spectra because diffusers are not used for radiance measurements and therefore they form a serious source of errors in trace gas retrievals. To cope with this problem, an additional averaged signal is generated from irradiance signals: subsequent measurements from a single sunset are averaged. This is called elevation averaging. Note that, since the CKD f_{relirr} is available (and the irradiance has thus been corrected for Sun elevation angle dependencies), this averaging operation is allowed. This algorithm step is only needed for the Solar_irradiance processing class.

24.7.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$\text{molm}^{-2}\text{nm}^{-1}\text{s}^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$\text{mol}^2\text{m}^{-4}\text{nm}^{-2}\text{s}^{-2}$
$S_{\text{irr,avg}}[\mathbf{x}_{\text{img}}]$	averaged signal	$\text{molm}^{-2}\text{nm}^{-1}\text{s}^{-1}$
$\sigma_{\text{irr,avg}}^2[\mathbf{x}_{\text{img}}]$	variance of averaged signal	$\text{mol}^2\text{m}^{-4}\text{nm}^{-2}\text{s}^{-2}$
N	number of measurements involved	1

24.7.2 Algorithm description and error propagation

The averaged irradiance signal is

$$S_{\text{irr,avg}}[\mathbf{x}_{\text{img}}] = \frac{1}{N} \sum_{i=1}^N S_i[\mathbf{x}_{\text{img}}] , \quad (257)$$

where N is the size of the subset of available Sun measurements that meets a restriction based on a certain elevation range.

24.7.3 Error propagation

The variance of the resulting averaged signal is

$$\sigma_{\text{irr,avg}}^2[\mathbf{x}_{\text{img}}] = \frac{1}{N^2} \sum_{i=1}^N \sigma_i^2[\mathbf{x}_{\text{img}}] . \quad (258)$$

24.8 Radiance responsivity

The radiance responsivity correction implements the relation between the charge (measured in electrons) as generated in the detector and the absolute incoming photon radiance (measured in $\text{mol s}^{-1} \text{m}^{-2} \text{nm}^{-1} \text{sr}^{-1}$). The total correction consists of two subsequent corrections. In this section, the so-called absolute radiance correction is performed. See Section 24.4 for details. Note that it is slightly artificial to define the absolute radiance for all pixels instead for the central row only (as dictated by the calibration measurements). However, the two-dimensional description enables us to cope with the spectral smile, if necessary. This algorithm step is only needed for the Earth_radiance processing class.

24.8.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$\text{e}^- \text{s}^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$\text{e}^{-2} \text{s}^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	$\text{mol m}^{-2} \text{nm}^{-1} \text{sr}^{-1} \text{s}^{-1}$
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} \text{sr}^{-2} \text{s}^{-2}$
$f_{\text{absrad}}[\mathbf{x}_{\text{det}}]$	conversion factor	$\text{mol m}^{-2} \text{nm}^{-1} \text{sr}^{-1} (\text{e}^-)^{-1}$
$s_{f_{\text{absrad}}}^2[\mathbf{x}_{\text{det}}]$	variance of conversion factor	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} \text{sr}^{-2} (\text{e}^-)^{-2}$

24.8.2 Algorithm description

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] \frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{absrad}}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}}. \quad (259)$$

The on-ground calibration provides the calibration key data $f_{\text{absrad}}[\mathbf{x}_{\text{det}}]$.

24.8.3 Error propagation

The radiometric responsivity calibration provides the calibration key data $s_{f_{\text{absrad}}}^2[\mathbf{x}_{\text{det}}]$. Because of the binning operation, knowledge about the correlations between individual uncorrelated radiance responsivity values in row direction is needed. For now, we assume the correlations are perfect, hence

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \left(\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{absrad}}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + S_i[\mathbf{x}_{\text{img}}]^2 s_{f_{\text{absrad}}}^2[\mathbf{x}_{\text{det}}]. \quad (260)$$

Here we again make use of the definition of the mean unbinned variance described in Section 20.4.2. If measurements show that signals in a row show a low correlation, then it may be possible to decrease the error.

24.9 Relative radiance responsivity

The relative radiance responsivity correction implements the second part of the relation between the charge (measured in electrons) as generated in the detector and the absolute incoming photon radiance (measured in $\text{mol s}^{-1} \text{m}^{-2} \text{nm}^{-1} \text{sr}^{-1}$). See Section 24.4 for details. This algorithm step is only needed for the Earth_radiance processing class.

24.9.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$\text{mol m}^{-2} \text{nm}^{-1} \text{sr}^{-1} \text{s}^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} \text{sr}^{-2} \text{s}^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	$\text{mol m}^{-2} \text{nm}^{-1} \text{sr}^{-1} \text{s}^{-1}$
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} \text{sr}^{-2} \text{s}^{-2}$
$f_{\text{relrad}}[\mathbf{x}_{\text{det}}]$	correction factor	1
$s_{f_{\text{relrad}}}^2[\mathbf{x}_{\text{det}}]$	variance of correction factor	1

24.9.2 Algorithm description

From the on-ground calibration, a CKD parameter f_{relrad} is provided that corrects the radiance in non-central rows.

$$S_o[\mathbf{x}_{\text{img}}] = S_i[\mathbf{x}_{\text{img}}] \frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{relrad}}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}}. \quad (261)$$

24.9.3 Error propagation

The on-ground calibration provides the calibration key data $s_{f,\text{relrad}}^2[\mathbf{x}_{\text{det}}]$.

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \left(\frac{\sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}} f_{\text{relrad}}[\mathbf{x}_{\text{det}}]}{N_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}}}} \right)^2 \sigma_i^2[\mathbf{x}_{\text{img}}] + S_i[\mathbf{x}_{\text{img}}]^2 \overline{s_{f,\text{relrad}}^2[\mathbf{x}_{\text{det}}]}. \quad (262)$$

Here we again make use of the definition of the mean unbinned variance described in Section 20.4.2.

24.10 Earth-Sun distance normalization

The spectral photon radiance provided is normalized to the average SI Earth-Sun distance of 1 Astronomical Unit (AU). If the Earth spectral radiance is denoted by S_e and the Earth-Sun distance by r_{es} , then the Earth spectral radiance normalized at 1 AU is given by:

$$S_e(r_{\text{au}}) = \left(\frac{r_{\text{es}}}{r_{\text{au}}} \right)^2 S_e(r_{\text{es}}), \quad (263)$$

where r_{au} is the Earth-Sun distance equal to 1 AU. Thus, the spectral photon radiance is normalized using the factor $\left(\frac{r_{\text{es}}}{r_{\text{au}}} \right)^2$. This algorithm is applied for both radiance *and* irradiance measurements.

24.10.1 Used parameters and symbols

Parameter	Description	Units
$S_i[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} before correction	$\text{mol m}^{-2} \text{nm}^{-1} (\text{sr}^{-1}) \text{s}^{-1}$
$\sigma_i^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} before correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} (\text{sr}^{-2}) \text{s}^{-2}$
$S_o[\mathbf{x}_{\text{img}}]$	signal in image pixel \mathbf{x}_{img} after correction	$\text{mol m}^{-2} \text{nm}^{-1} (\text{sr}^{-1}) \text{s}^{-1}$
$\sigma_o^2[\mathbf{x}_{\text{img}}]$	signal variance in image pixel \mathbf{x}_{img} after correction	$\text{mol}^2 \text{m}^{-4} \text{nm}^{-2} (\text{sr}^{-2}) \text{s}^{-2}$
r_{es}	Earth-Sun distance at the time of the measurement	m
r_{au}	Average SI Earth-Sun distance; 1 AU = 149597870700	m

24.10.2 Algorithm description

$$S_o[\mathbf{x}_{\text{img}}] = \left(\frac{r_{\text{es}}}{r_{\text{au}}} \right)^2 S_i[\mathbf{x}_{\text{img}}] \quad (264)$$

24.10.3 Error propagation

$$\sigma_o^2[\mathbf{x}_{\text{img}}] = \left(\frac{r_{\text{es}}}{r_{\text{au}}} \right)^4 \sigma_i^2[\mathbf{x}_{\text{img}}] \quad (265)$$

Part VI

Annotation

The preceding sections all deal with how electromagnetic radiation is recorded by the instrument's detectors. In order to use such data however, it is necessary to know the context in which the measurements were performed. When did the measurement take place? What are the coordinates of the ground pixels? Under which angles was the radiation scattered by the atmosphere? Did any errors occur during the processing? Answers to such questions are given by a number of dedicated algorithms and added to the Level-1B products as annotation data.

25 Time bases and conversions

Obviously, time constitutes one of the most important pieces of annotation data. Therefore, all measurements in the TROPOMI Level-1B products will be augmented with a timestamp that indicates when the measurement was taken. The time of a measurement is also one of the main inputs to the geometrical algorithms. Depending on the algorithm, different time bases are needed and conversions between these time bases are required. The L01b Processor has support for the time bases described in Table 13. The different time types that are used in Table 13 are described in Table 14. All the times are relative to a specific epoch. This is necessary in order to be able to correlate the different time types and time bases and convert from one to another. The epochs that are used are described in Table 15.

Time base	Symbol	Unit	Epoch
CCSDS Unsegmented time Code (CUC)	t_{cuc}	s	2000-01-01 (TAI)
UTC since 2010	$t_{utc,2010}$	s	2010-01-01 (UTC)
UTC since 1970	$t_{utc,1970}$	s	1970-01-01 (UTC)
TAI since 2010	$t_{tai,2010}$	s	2010-01-01 (UTC)
TAI since J2000.0	$t_{tai,J2000}$	s	J.2000.0
UT1 since 2010	$t_{ut1,2010}$	s	2010-01-01 (UTC)
UT1 since J2000.0	$t_{ut1,J2000}$	s	J.2000.0
TT since J2000.0	$t_{tt,J2000}$	s	J.2000.0
Julian Date (JD) J2000.0	J_{J2000}	JD	J.2000.0

Table 13: Time bases of the TROPOMI L01b Processor, their unit and epoch.

UT1 time follows the rotation of the Earth as closely as possible. As the duration of a solar day (i.e. the time for one full revolution of the Earth) is slightly larger than 86400 seconds, UT1 drifts in relation to TAI and UTC. The exact rotation of the Earth is monitored by the International Earth Rotation and Reference Systems Service (IERS). The difference between UTC and UT1 is published by the IERS in Bulletin B. A long-term overview of the difference between UT1 and UTC is given in Figure 49. The L01b Processor will read the IERS Bulletin-B data products and use the data for conversion of time from UTC and TAI to UT1:

$$t_{ut1,2010} = t_{utc,2010} + T_{ut1-utc}(t_{utc,2010}), \quad (266a)$$

$$t_{ut1,J2000} = t_{utc,J2000} + T_{ut1-utc}(t_{utc,J2000}), \quad (266b)$$

where $T_{ut1-utc}(t_{utc})$ is the difference between UT1 and UTC for a UTC timestamp t_{utc} . As the difference between UT1 and UTC is always less than a second and the drift between UT1 and UTC is relatively slow, the same value is used for converting back to UTC, using the UT1 timestamp as a UTC timestamp. The corresponding error in the conversion is neglected:

$$t_{utc,2010} = t_{ut1,2010} - T_{ut1-utc}(t_{ut1,2010}), \quad (267a)$$

$$t_{utc,J2000} = t_{ut1,J2000} - T_{ut1-utc}(t_{ut1,J2000}). \quad (267b)$$

To keep the difference between UT1 and UTC within 1 seconds, leap seconds are introduced, which are published in IERS Bulletin C. These leap seconds need to be taken into account for conversions from the TAI

Time type	Description
CCSDS unsegmented time code (CUC)	Seconds since an epoch; identical to TAI. CUC times are used in the S5p telemetry and science data.
Coordinated universal time (UTC)	The primary time standard by which the world regulates clocks and time. UTC times in seconds do not include leap seconds. UTC time is generally used for presenting time in a human readable format.
International atomic time (TAI)	High-precision atomic coordinate time standard based on the notional passage of proper time on Earth's geoid. It is the basis for coordinated universal time (UTC), which is used for civil timekeeping all over the Earth's surface, and for terrestrial time, which is used for astronomical calculations. TAI timestamps are used in the L01b internally where possible, as they are the most convenient to work with.
Universal time (UT1)	Time scale based on the rotation of the Earth. UT1 is the same everywhere on Earth, and is proportional to the rotation angle of the Earth with respect to distant quasars, specifically, the international celestial reference frame (ICRF), neglecting some small adjustments. Time in UT1 is needed for carrying out certain reference frame transformations.
Terrestrial time (TT)	Astronomical time standard defined by the International Astronomical Union (IAU), primarily for time measurements of astronomical observations made from the surface of the Earth. Time in TT1 is needed for carrying out certain reference frame transformations.
Julian date (JD)	The Julian day number for the preceding noon plus the fraction of the day since that instant. Julian dates are expressed as a Julian day number with a decimal fraction added. The Julian day number (JDN) is the integer assigned to a whole solar day in the Julian day count starting from noon Greenwich mean time, with Julian day number 0 assigned to the day starting at noon on January 1, 4713 BC proleptic Julian calendar. (November 24, 4714 BC in the proleptic Gregorian calendar.) A Julian day is defined as 86400 s.

Table 14: Time types of the TROPOMI L01b Processor

Time epoch	Description
2000-01-01 (TAI)	This epoch is used for the time stamps in the S5p telemetry and science data.
1970-01-01 (UTC)	Epoch for the Unix clock and C times functions.
2010-01-01 (UTC)	Internal epoch for the TROPOMI L01b Processor. Most time conversions in the L01b Processor use this epoch as a common basis. This means that for time conversion a time is first converted to this epoch as an intermediate step.
J2000.0	The current standard epoch for astronomical calculations as designated by the International Astronomical Union (IAU). The J2000.0 epoch corresponds to: <ol style="list-style-type: none"> 1. The Julian date 2451545.0 TT (Terrestrial Time). 2. January 1, 2000, 11:59:27.816 TAI (International Atomic Time). 3. January 1, 2000, 11:58:55.816 UTC (Coordinated Universal Time).

Table 15: Time epochs of the TROPOMI L01b Processor

time base to the UTC time base. Leap seconds are announced by the IERS and published in the IERS Bulletin C. The L01b Processor will read these Bulletin-C data products to build a table containing all announced leap seconds. This table is used for the time conversions in the L01b Processor. The leap seconds up to 2012 are shown in Table 16.

To convert from TAI to UTC and vice-versa in the same epoch:

$$t_{tai,2010} = t_{utc,2010} + T_{leapsec,utc}(t_{utc,2010}), \quad (268a)$$

$$t_{utc,2010} = t_{tai,2010} - T_{leapsec,tai}(t_{tai,2010}), \quad (268b)$$

where $T_{leapsec,utc}(t_{utc})$ and $T_{leapsec,tai}(t_{tai})$ are the number of leap seconds for a UTC timestamp t_{utc} and that for a

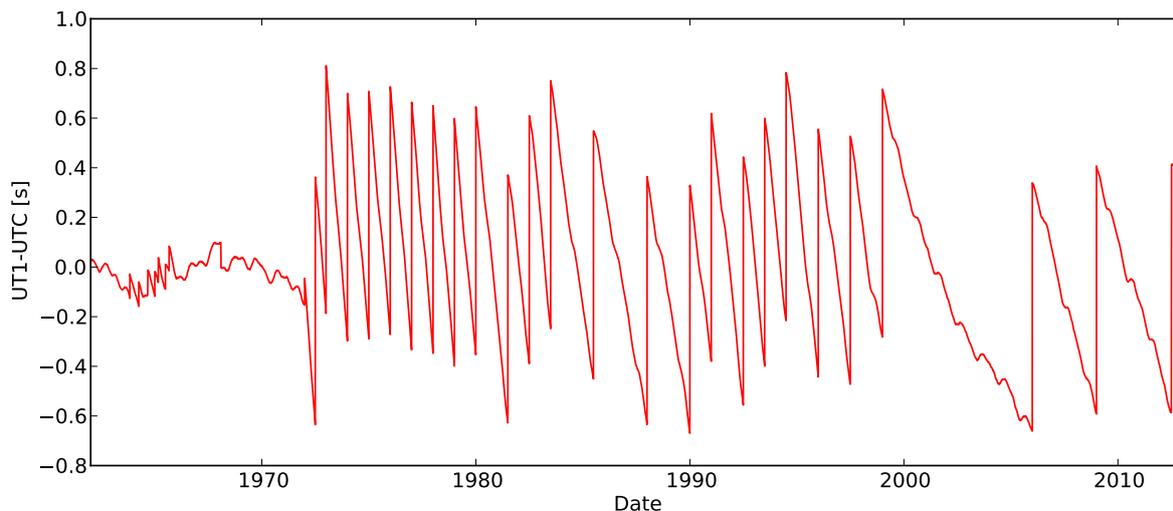


Figure 49: Long term difference between UT1 and UTC.

Starting from	Leap seconds	Starting from	Leap seconds
1972-01-01 00:00:00 UTC	10	1985-07-01 00:00:00 UTC	23
1972-07-01 00:00:00 UTC	11	1988-01-01 00:00:00 UTC	24
1973-01-01 00:00:00 UTC	12	1990-01-01 00:00:00 UTC	25
1974-01-01 00:00:00 UTC	13	1991-01-01 00:00:00 UTC	26
1975-01-01 00:00:00 UTC	14	1992-07-01 00:00:00 UTC	27
1976-01-01 00:00:00 UTC	15	1993-07-01 00:00:00 UTC	28
1977-01-01 00:00:00 UTC	16	1994-07-01 00:00:00 UTC	29
1978-01-01 00:00:00 UTC	17	1996-01-01 00:00:00 UTC	30
1979-01-01 00:00:00 UTC	18	1997-07-01 00:00:00 UTC	31
1980-01-01 00:00:00 UTC	19	1999-01-01 00:00:00 UTC	32
1981-07-01 00:00:00 UTC	20	2006-01-01 00:00:00 UTC	33
1982-07-01 00:00:00 UTC	21	2009-01-01 00:00:00 UTC	34
1983-07-01 00:00:00 UTC	22	2012-07-01 00:00:00 UTC	35

Table 16: Leap seconds up to 2012. The leap seconds specify the time difference in seconds between TAI and UTC. At the introduction of leap seconds in 1972, this difference already amounted to 10 seconds.

TAI timestamp t_{tai} respectively.

For conversion of a UTC timestamp to a different epoch, it is sufficient to add or subtract the difference in seconds between the epochs. So, to convert between epochs:

$$t_{\text{utc},1970} = t_{\text{utc},2010} + \Delta T_{\text{epoch,utc}}[2010, 1970] , \quad (269a)$$

$$t_{\text{utc},2010} = t_{\text{utc},1970} + \Delta T_{\text{epoch,utc}}[1970, 2010] , \quad (269b)$$

where $\Delta T_{\text{epoch,utc}}[t_1, t_2]$ is the number of UTC seconds between two epochs t_1 and t_2 . Here we use the convention that $\Delta T_{\text{epoch,utc}}[t_1, t_2]$ is positive for $t_1 > t_2$. The various ΔT_{epoch} 's have the following values:

$$\Delta T_{\text{epoch,utc}}[2010, 1970] = 14610 \cdot 86400 \text{ s} , \quad (270a)$$

$$\Delta T_{\text{epoch,utc}}[1970, 2010] = -14610 \cdot 86400 \text{ s} . \quad (270b)$$

CUC time is essentially a TAI time, but it has a TAI time as epoch, where the internal TAI time representation for the L01b uses a UTC epoch. For converting the CUC time to the internal TAI time, the time must therefore

be corrected for the epoch as well as leap seconds:

$$t_{\text{cuc}} = t_{\text{tai},2010} + \Delta T_{\text{epoch,utc}}[2010,2000] + T_{\text{leapsec}}[2010], \quad (271a)$$

$$t_{\text{tai},2010} = t_{\text{cuc}} + \Delta T_{\text{epoch,utc}}[2000,2010] - T_{\text{leapsec}}[2010], \quad (271b)$$

where $\Delta T_{\text{epoch,utc}}[t_1, t_2]$ is the number of UTC seconds between two epochs t_1 and t_2 and $T_{\text{leapsec}}[t]$ is the total number of leap seconds at epoch t . Here we use the convention that $\Delta T_{\text{epoch,utc}}[t_1, t_2]$ is positive for $t_1 > t_2$. These parameters have the following values:

$$\Delta T_{\text{epoch,utc}}[2010,2000] = 3653 \cdot 86400 \text{ s}, \quad (272a)$$

$$\Delta T_{\text{epoch,utc}}[2000,2010] = -3653 \cdot 86400 \text{ s}, \quad (272b)$$

$$T_{\text{leapsec}}[2010] = 34 \text{ s}. \quad (272c)$$

The difference between TAI and TT is a fixed offset $\Delta T_{\text{tai,tt}}$, which is independent of the epoch:

$$t_{\text{tt},J2000} = t_{\text{tai},J2000} + \Delta T_{\text{tai,tt}}, \quad (273a)$$

$$t_{\text{tai},J2000} = t_{\text{tt},J2000} - \Delta T_{\text{tai,tt}}, \quad (273b)$$

$$\Delta T_{\text{tai,tt}} = 32.184 \text{ s}. \quad (273c)$$

To retain the fixed offset between TAI and TT, this offset is not applied when converting a TAI time to or from the J2000.0 epoch. The fact that J2000.0 starts at noon rather than midnight will need to be accounted for. Conversion of TAI time to the J2000.0 epoch is as follows:

$$t_{\text{tai},J2000} = t_{\text{tai},2010} + \Delta T_{\text{epoch,utc}}[2010,2000] - 0.5 \cdot 86400 + T_{\text{leapsec}}[2010], \quad (274a)$$

$$t_{\text{tai},2010} = t_{\text{tai},J2000} + \Delta T_{\text{epoch,utc}}[2000,2010] + 0.5 \cdot 86400 - T_{\text{leapsec}}[2010], \quad (274b)$$

with

$$\Delta T_{\text{epoch,utc}}[2010,2000] = 3653 \cdot 86400 \text{ s}, \quad (275a)$$

$$\Delta T_{\text{epoch,utc}}[2000,2010] = -3653 \cdot 86400 \text{ s}. \quad (275b)$$

Julian Date (JD) J_{J2000} is based on Terrestrial Time (TT) and in the same epoch J2000.0, so deriving J_{J2000} from $t_{\text{tt},J2000}$ is straightforward:

$$J_{J2000} = \frac{t_{\text{tt},J2000}}{86400}, \quad (276a)$$

$$t_{\text{tt},J2000} = J_{J2000} \cdot 86400. \quad (276b)$$

26 Geometrical definitions

For the geometrical algorithms that will be described in Section 27, a number of geometrical definitions need to be explained first. These consist of reference frames, reference frame transformations, and optical functions.

26.1 Reference frame definitions

The reference frames needed to define the positions, velocities and angles of the following geolocation calculations will be explained in this section. Most definitions have been adopted, modified and combined from [RD4], as well as other industry documents, unless stated otherwise.

26.1.1 WGS84 Earth reference ellipsoid

To simulate the geometry of the Earth, the WGS84 Earth reference ellipsoid is used. This ellipsoid is created by rotating the ellipse of Figure 50 about the axis of rotation (making it in effect an oblate spheroid or ellipsoid of revolution). The ellipse is defined as having a semi-major axis a (equatorial radius) of 6378137.0 m and the flattening $f = (a - b)/a$ of the ellipse is defined as 1/298.257223563 [RD13]. This results in a semi-minor axis b (polar radius) of 6356752.3142 m. Locations on the ellipsoid may be expressed as geocentric or geodetic coordinates. The axes cross at the center point (origin) of the ellipse, which is the center of mass of the Earth.

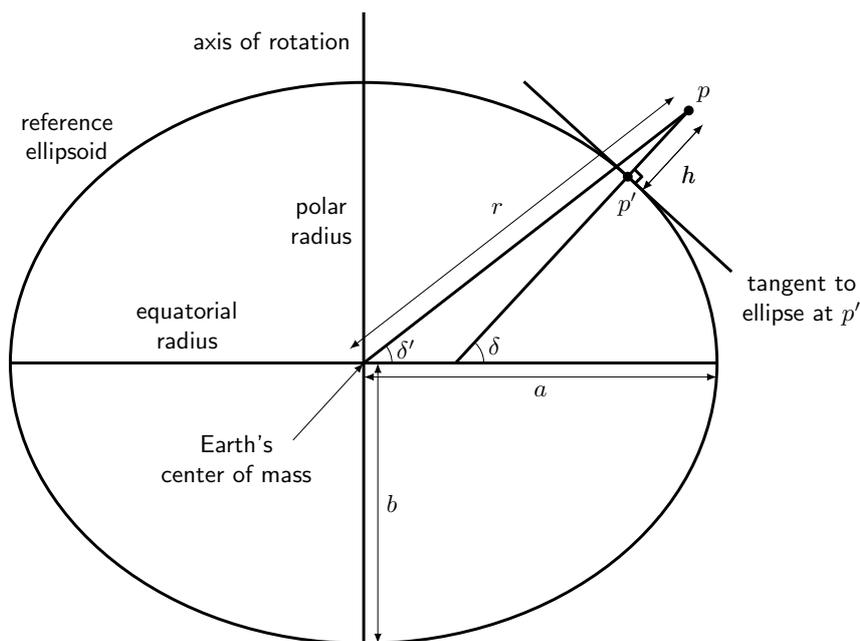


Figure 50: Geocentric versus geodetic coordinates with respect to the WGS84 Earth reference ellipsoid.

Geocentric coordinates are defined with respect to this center of mass of the Earth. This can be either in Cartesian coordinates (x, y, z) or spherical coordinates (δ', ϑ, r) , defined as geocentric latitude, longitude and radius (see Figure 50). In the latter, the longitude ϑ is measured positive eastwards from the IERS reference meridian (Greenwich, see also Figure 52).

In contrast, the geodetic coordinates (δ, ϑ, h) : geodetic latitude, longitude and altitude, respectively) that are used in the output Level-1b data for locations on Earth, are defined with respect to the WGS84 Earth reference ellipsoid. The longitude in the geodetic system is the same as for the geocentric system, and therefore has the same name and symbol in both systems. However, the geodetic latitude is defined by the angle of the normal from point P to the Earth reference ellipsoid and the equatorial plane. The altitude h is the distance from the point P measured perpendicular to the plane tangent to the Earth reference ellipsoid.

26.1.2 Inertial reference frame

The inertial reference frame is the geocentric mean-of-date reference frame at epoch J2000.0, with its:

- Origin at the center of mass of the Earth at epoch J2000.
- Z-axis in the direction of Earth's mean rotation axis at epoch J2000, pointing north.
- X-axis in the direction of the mean vernal equinox at epoch J2000.
- Y-axis completing the right-handed orthogonal Cartesian coordinate system.

The vernal equinox is the intersection of the Earth's mean equator plane with the mean ecliptic, while the ecliptic is the orbital plane of the Earth around the Sun. The X-Y plane thus coincides with the predicted mean Earth equatorial plane, at the epoch J2000.0. Here, the word 'mean' indicates that the relatively short periodic nutation of the Earth, is smoothed out in the calculation of the mean equator and equinox. That is, only the mean precession of the Earth is taken into account.

This reference frame is based (in accordance with the recommendations of the International Astronomical Union (IAU)) on the Fifth Fundamental Star Catalog (FK5) for the epoch J2000.0, since the directions of its axes are defined relative to a given number of the FK5 catalog's positions and proper motions. The accuracy of this reference system, realized through FK5, is approximately 0.1 arcseconds. Figure 51 depicts a schematic of the inertial reference frame.

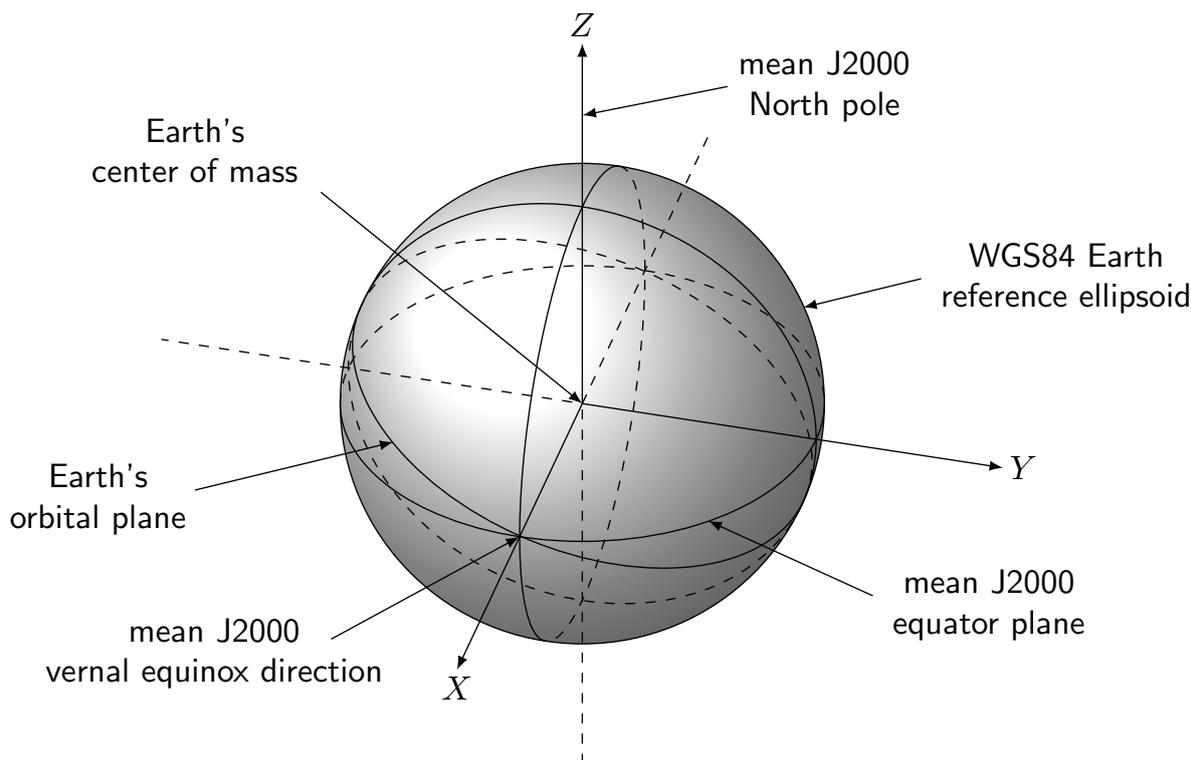


Figure 51: Definition of the inertial reference frame.

26.1.3 Mean-of-date reference frame

The mean-of-date reference frame has the same definition for its axes as the inertial reference frame. However, the coordinate axes of the system are now rotated with the Earth's precession from J2000.0, to the date used as epoch. The precession of the Earth is the secular effect of the gravitational attraction from the Sun and the Moon on the Earth's equatorial bulge (see also Section 26.2.5). Here, the expression 'mean' indicates that the relatively short periodic nutation of the Earth is smoothed out, in the calculation of parameters for that epoch.

26.1.4 True-of-date reference frame

The true-of-date reference frame also has the same definition for its axes as the inertial reference frame. In this case, however, the coordinate axes of this system are rotated with the Earth's precession *and* nutation from J2000.0, to the date used as epoch. Nutation is the short periodic effect of the gravitational attraction of the Moon and, to a lesser extent, other celestial bodies, on the Earth's equatorial bulge (see also Section 26.2.5). The expression 'true' indicates the usage of the true instantaneous Earth equatorial plane and vernal equinox, thus, no averaging of effects takes place.

26.1.5 Earth-fixed reference frame

The Earth-fixed reference frame in use is the IERS terrestrial reference frame (ITRF). The zero longitude ϑ_0 or IERS reference meridian, as well as the IERS reference pole (that define the ITRF), are maintained by the International Earth Rotation and Reference Systems Service (IERS), and are based on a large number of observing stations. This coordinate system is connected to, and rotates with the Earth, so velocities expressed in this coordinate system include the rotation of the Earth. Furthermore it is also connected to the WGS84 Earth reference ellipsoid. Precession, nutation, rotation about the pole, as well as the polar motion, are all taken into account (see also Section 26.2.5). The axes are defined as follows:

- The origin is the center of mass of the Earth (i.e., the center of the WGS84 Earth reference ellipsoid).
- The positive Z-axis goes out the north pole (i.e., the semi-minor axis of the WGS84 Earth reference ellipsoid).

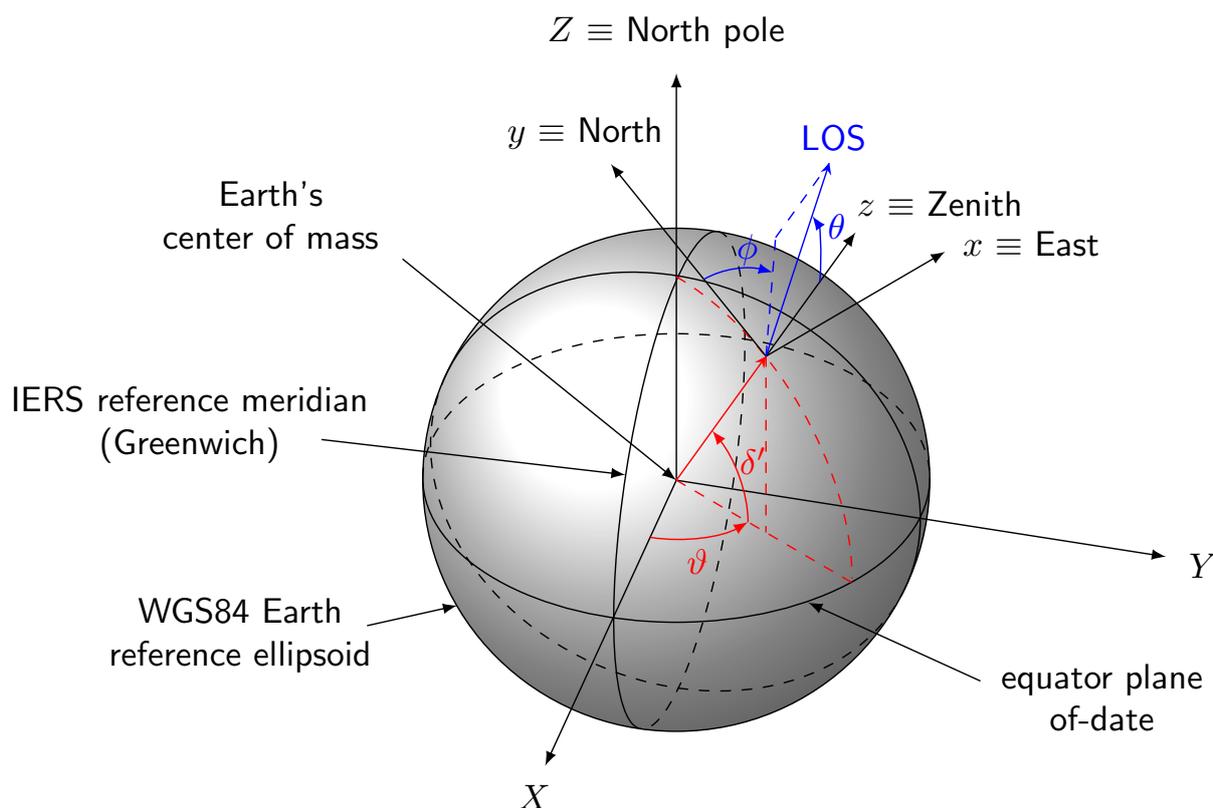


Figure 52: Definition of the Earth-fixed reference frame indicated by (X, Y, Z) , including its longitude ϑ and geocentric latitude δ' angles, as well as the topocentric reference frame indicated by (x, y, z) , with its topocentric azimuth ϕ and zenith θ angles.

- The X - Y plane is the equatorial plane (i.e., the plane spanned by the rotated semi-major axis in the WGS84 Earth reference ellipsoid).
- The X -axis is along the prime meridian (Greenwich; zero point of longitude ϑ_0).
- The Y -axis is then set to make the system right-handed. This results in the axis pointing through the Indian Ocean.

This definition is depicted in Figure 52, in which also the longitude ϑ and geocentric latitude δ' angles are indicated. Note that the WGS84 coordinate system as defined in [RD13] is *not* used, as it depends on the IERS reference meridian at epoch 1984, which is outdated.

26.1.6 Topocentric reference frame

The topocentric reference frame is attached to the Earth's surface. For the topocentric reference frame:

- The origin is defined by any longitude ϑ and latitude δ in the Earth-fixed reference frame, on the surface of the WGS84 Earth reference ellipsoid.
- The Z -axis coincides with the normal vector to the Earth reference ellipsoid, positive towards zenith (away from the Earth).
- The X - Y plane is the plane orthogonal to the Z -axis, and thus tangent to the Earth reference ellipsoid.
- The X -axis points towards east.
- The Y -axis points towards north.

This is shown in Figure 52, in which also the topocentric azimuth ϕ and zenith θ angles, that define a direction vector in this frame, are indicated.

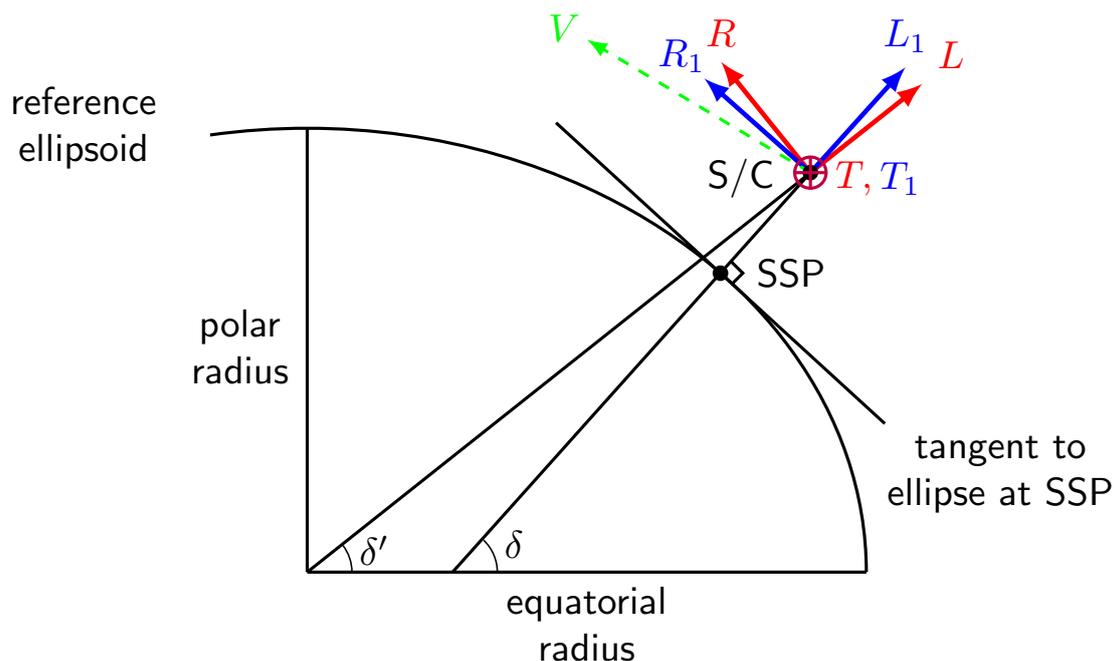


Figure 53: Local orbital reference frame (red) versus local relative orbital reference frame (blue) definition. The velocity vector V (green) is in the same plane as the R - L plane.

26.1.7 Local orbital reference frame

The position of the local orbital reference frame is defined by the position of the spacecraft, while the orientation is independent of the attitude of the spacecraft:

- The origin of the local orbital reference frame (T, R, L) is the satellite in-flight center of mass.
- The L -axis points in the direction opposite to the Earth's center.
- The R -axis is perpendicular to the L -axis and in the vertical plane containing V such that $\cos(\mathbf{V}, \hat{\mathbf{r}}) > 0$, where \mathbf{V} is the absolute velocity vector and $\hat{\mathbf{r}}$ is the unit vector in the direction of the R -axis.
- The T -axis completes the right-handed frame, ($\hat{\mathbf{t}} = \hat{\mathbf{r}} \times \hat{\mathbf{l}}$).

26.1.8 Local relative orbital reference frame

The local relative orbital reference frame (T_1, R_1, L_1) has a similar definition as the local orbital reference frame except for local normal pointing, i.e. the unit vector L_1 is parallel to the local normal of the WGS84 Earth reference ellipsoid, directed upward and crossing the spacecraft in-flight center of mass and the unit vector R_1 is in the plane containing the velocity vector in the Earth-fixed frame. This attitude is also known as local normal pointing (LNP).

The definitions of, and the relation between, the local orbital reference frame and local relative orbital reference frame are visualized in Figure 53.

26.1.9 Spacecraft reference frame

The spacecraft reference frame is defined with respect to the actual hardware of the spacecraft, i.e. it is "attached" to the spacecraft. In this way, it is possible to express the orientation of the spacecraft with respect to the inertial reference frame. The following definition of this reference frame is adopted from the EADS Astrium implementation, which is also used by Dutch Space:

- The origin is located at the interface plane separating the satellite and the launcher, at the center of the adaptor.

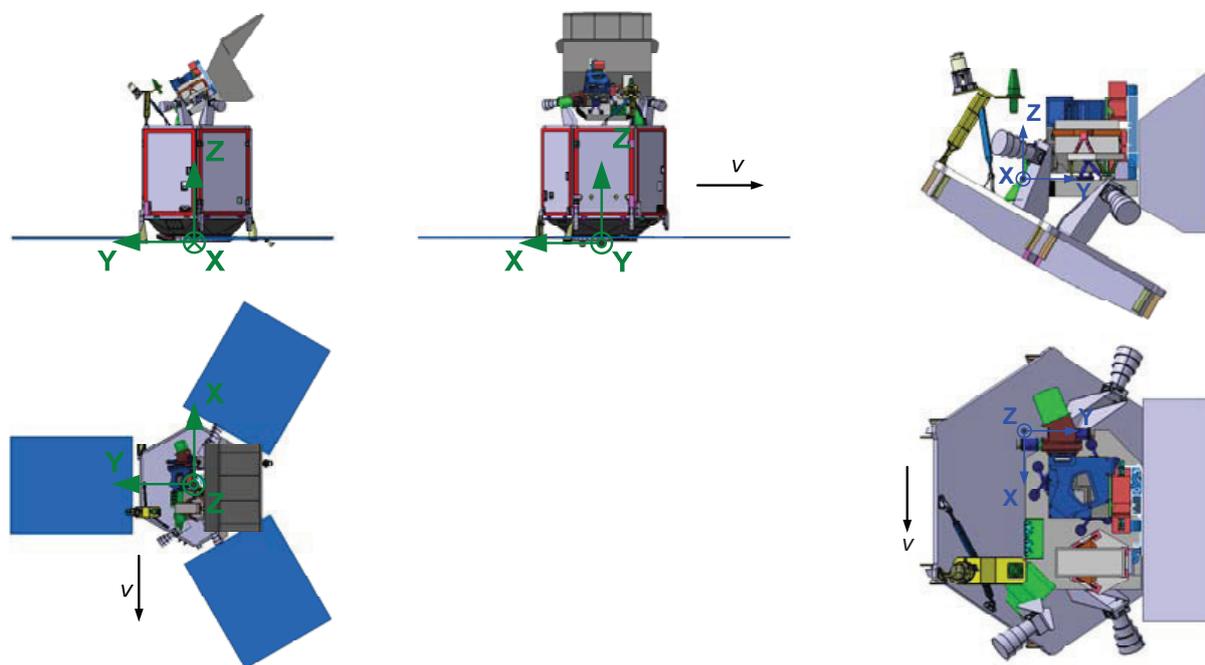


Figure 54: Definition of the spacecraft (left) and payload (right) reference frames with respect to their hardware. Note that the right figures of the payload have a roll angle of 30 degrees with respect to the left figures of the spacecraft reference frame.

- The Z_S axis is normal to the launcher interface plane, towards the body of the satellite.
- The Y_S axis points towards a solar panel. For ease, the deep space wall is taken as $-Y_S$.
- The X_S axis completes a right-handed orthogonal set. It results that $+X_S$ is pointing in the opposite direction to the velocity vector.

Although this definition deviates from the ESA requirements, it is the version used throughout this document, as it is EADS Astrium that will supply the attitude information of this reference frame with respect to the inertial reference frame. In the left part of Figure 54 one can see a visualization of the above definition.

The spacecraft reference frame holds a constant in-flight approximate orientation with respect to the inertial reference frame. It will try to control its attitude within certain boundary angles to align with the LNP attitude, which is exactly opposite to the local relative orbital reference frame, the coordinates of the latter being in a different order: (X_S, Y_S, Z_S) versus (R, T, L) . This is defined as the Z_S axis pointing towards the center of the Earth, while the X_S axis is perpendicular to the Z_S , in the orbital plane and opposite to the velocity vector V . The Y_S then completes the orthogonal set pointing normal to the orbital plane. This alignment only holds true when the spacecraft has the ideal LNP attitude, which will never exactly occur in practice, but is the goal of the attitude control subsystem; in practice the attitude of the spacecraft will be misaligned with the local relative orbital reference frame within certain maximum allowed angles.

The in-flight attitude of the spacecraft reference frame with respect to the inertial reference frame will be constantly measured at certain time instances by the on-board star tracker (STR) system, and defined in unit quaternions $\mathbf{q} = [q_0, q_1, q_2, q_3]$. The STR system makes images in three orthogonal directions using a relatively small field-of-view and compares these to a nearly constant map of the star sky. This is used to determine the orientation of the spacecraft.

The spacecraft alignment cube (SAC) will be aligned with this reference frame, and act as a reference for the integration alignment measurements. The SAC will then be the practical implementation and definition of the spacecraft reference frame for the geolocation calculations.

26.1.10 Payload reference frame

The spacecraft supplier's implementation (in accordance with ESA requirements [RD4]) of the payload reference frame (X_P, Y_P, Z_P), which is also used by the instrument prime contractor, as shown in the right part Figure 54, is defined as:

- The origin is located at the center of the UVN nadir entrance slit.
- The Z_P -axis is parallel to the instrument boresight, and is aligned with $-\mathbf{L}_1$ (of the local relative orbital reference frame).
- The Y_P -axis is parallel to the larger dimension of the entrance slit.
- The X_P -axis completes a right-handed orthogonal set and points in the same direction as the velocity vector relative to the Earth-fixed WGS84 Earth reference ellipsoid.

Although the ESA SRD calls this frame the payload reference frame, it is also called instrument reference frame by other parties and in other documents. The optical alignment cube (OAC) will be aligned with this reference frame, and act as a reference for the line-of-sight angle measurements. The OAC will then be the practical implementation and definition of the payload reference frame for the geolocation calculations.

The payload (the TROPOMI instrument) is designed and built at a different place (Dutch Space) than the spacecraft bus (EADS Astrium), and after calibration and testing, they will be integrated before launch. Since no mechanical part can be integrated and aligned perfectly to their designed position and orientation before launch, misalignment errors are expected. Therefore, the orientation of the integrated payload will be measured with respect to the spacecraft bus, by using theodolites to test the alignment between the OAC and the SAC.

26.1.11 Azimuth and elevation definition

The line-of-sight angles of the detector pixels are measured by rotating the instrument about two axes on a cradle, such that the collimated beam from a star stimulus falls under different angles on the entrance slit. The cradle will rotate about one axis (the X -axis of the payload reference frame), such that one of the two angles is traversed in the plane tangent to the length of the entrance slit, which is in swath direction. It will furthermore rotate about another orthogonal axis (the Y -axis of the payload reference frame), such that the other angle varies orthogonal to that plane, which is the elevation angle in the direction of the velocity vector of the spacecraft. The cradle angles which are controlled are the tip-tilt and rotation angles. The accurate conversion of these angles to azimuth and elevation angles can be done after the alignment measurements.

The most common definition for azimuth and elevation in a right-handed Cartesian X, Y, Z reference frame is where the elevation angle is measured from the X - Y plane towards the Z -axis (range $-\pi/2$ - $+\pi/2$), while the azimuth angle is defined from the X -axis towards the Y -axis (sometimes vice-versa), rotating about the Z -axis (range $-\pi$ - $+\pi$ or 0 - 2π). However, if this definition would be employed in the previously defined payload reference frame for measuring the pixel line-of-sight angles of the TROPOMI instrument, by just rotating in the swath direction, the azimuth angle would alternate between $-\pi$ and π , while the elevation would vary between 0 and π for both alternations. Then by also rotating in the along track direction, both the azimuth and the elevation angle would vary. This common definition for the azimuth and elevation thus does not seem convenient in the defined payload reference frame.

Concluding from the discussion above, a convenient definition for the the azimuth angle is by rotating about the X -axis, from the Z -axis towards the $-Y$ -axis, so that the definition for the elevation angle then follows as rotating about Y -axis, from the Z -axis towards the X -axis (or rather: from the Y - Z -plane towards the X -axis). In this way, when changing the angle in swath direction, the azimuth angle will vary from 0 towards the positive and negative numbers (from about -59 to $+59$ degrees to span the entire field of view). When changing the angle in velocity direction, the elevation will vary from 0 towards the positive and negative numbers (up to about -8 or $+8$ degrees to span the field of view accounting for the spatial smile effect).

This definition is illustrated in Figure 55, and is the definition for the LOS angles in the payload reference frame adopted in the geolocation calculations. Converting the cradle angles to the payload reference frame LOS angles using the alignment of the cradle alignment cube, the instrument alignment cube, and the star stimulus collimator cube, is considered out-of-scope for this document.

26.1.12 Sun port reference frame

The Sun port reference frame is defined with respect to the Sun diffuser aperture, which is defined by the inner vane of the Sun port baffle:

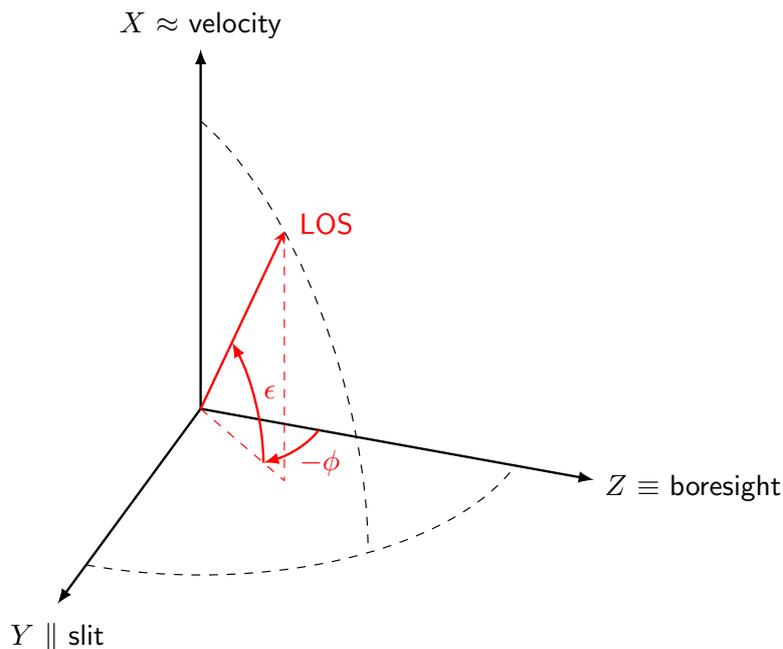


Figure 55: Negative azimuth ϕ and positive elevation ϵ angle definition of the line of sight with respect to the payload reference frame.

- The origin is located at the center of the inner vane of the Sun port baffle.
- The X -axis is parallel to the Z -axis of the Payload reference frame.
- The Z -axis has an azimuth offset angle (AZO) of 23.75 deg with the normal to the inner vane plane, rotated about the above defined X -axis.
- The Y -axis completes a right-handed orthogonal set and is thus makes an angle of 23.75 deg with the Y_P -axis of the payload reference frame.

To define the direction of the Sun with respect to the Sun port reference frame, an azimuth and elevation angle are defined. These angles have a similar definition as the Earth port azimuth and elevation angles explained above, but now with respect to the Sun port reference frame instead of the payload reference frame.

26.1.13 Structural Deformation

Due to temperature variations in the structure of the satellite during its lifetime, and deviation with respect to the temperature of the structure during the calibration testing on-ground, deformations occur, which result in a different in-orbit orientation of the payload with respect to the spacecraft as during on-ground calibration. The deformation of the top-floor of the satellite to which the TSS is attached with three isostatic bi-pods results in the largest alignment errors. The star trackers are also attached to this top-floor, while the payload (TROPOMI) is attached to the TSS.

The top-floor of the satellite box-like structure has a hexagonal shape attached to six stiffeners to which six side panels are attached, see Figure 54. This structure is thus statically overdetermined, and the thermal deformational due to temperature variations in this top-floor is a complex process, which can only be analysed by finite elements methods.

The error in roll (across-track) of the payload is largest and can be predicted more accurately than the yaw and pitch errors. The correlation between the top-floor temperature and the roll error is sufficient enough in order to correct this error, while for the pitch and yaw angles this correlation is too complex and an attempt at a correction there will most probably lead to worse results. Thus, only the roll error is corrected for, which will be elaborated in Section 26.2.1.

Furthermore, the deformation internal to the TSS structure, is within the instrument pointing knowledge budget, and thus not corrected for. In addition, it is to be determined whether the gravity-release deformation needs to be corrected (both for the top floor and TSS), or falls within the pointing knowledge error budget.

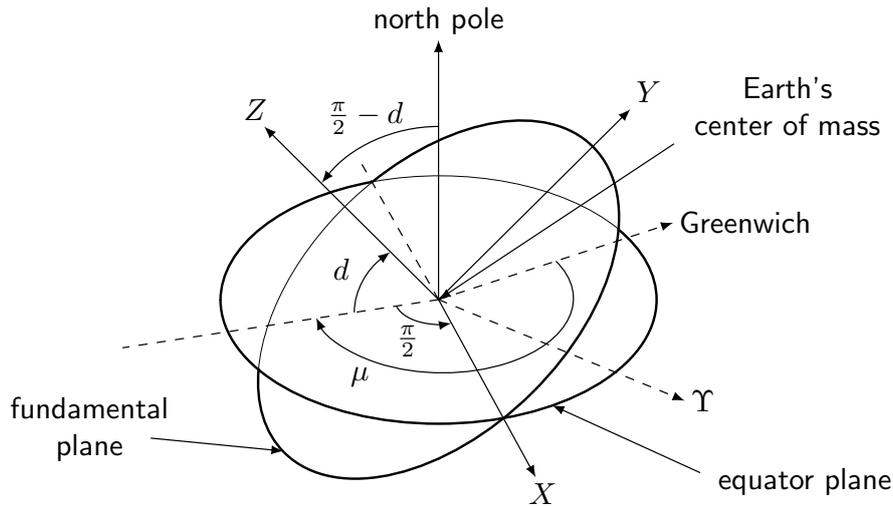


Figure 56: Solar eclipse fundamental reference frame definition. The geocentric equatorial declination angle d and the Greenwich Hour Angle μ of the Z-axis of the fundamental reference frame, describe the orientation of the frame with respect to the Earth-fixed reference frame. Greenwich here lies in the direction of the Greenwich reference meridian on the Equator plane.

26.1.14 Fundamental reference frame

For solar eclipse geometry purposes, the eclipse shadow axis is defined as the line between the center of the Sun and the center of the Moon. The fundamental reference frame relates to this axis, and is defined as follows:

- The origin is located at the center of the Earth.
- The Z-axis is parallel to the eclipse shadow axis, positive towards the Moon.
- The X-axis passes through the Earth's equator and is positive toward the East.
- The Y-axis complements the orthogonal right-handed reference frame and is positive towards the North.
- The XY-plane is called the fundamental plane.

The definition is illustrated in Figure 56. The reference frame is chosen in this way, such that the eclipse penumbral, umbral and/or antumbral shadows are always defined by two concentric circles in the fundamental frame, about the shadow's axis.

26.2 Reference frame transformations

To convert coordinates (that can for instance be based on positions or line-of-sight unit vectors) between the reference frames defined in Section 26.1, reference frame transformations are needed. These are based on a rotation matrix, where one definition of a reference frame is rotated with respect to another, and a translation vector, where the origin of one frame has a fixed offset to the other. Following up on this section, are the description of the geometrical algorithms, which refer back to parts of this section in their calculation steps.

26.2.1 Payload reference frame to spacecraft reference frame

In accordance with Figure 54, noting a roll angle of 30 degrees between the two frames, the design rotation between payload reference frame and the spacecraft reference frame is given as

$$\mathbf{R}_{zyx, PRF \rightarrow SRF} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -\cos \frac{\pi}{6} & +\sin \frac{\pi}{6} \\ 0 & +\sin \frac{\pi}{6} & +\cos \frac{\pi}{6} \end{bmatrix}. \quad (277)$$

The transformation of a point $\mathbf{q} = [x, y, z]$ from the payload reference frame to the spacecraft reference frame can then be evaluated as

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix}_{\mathbf{q}_{\text{SRF}}} = \mathbf{R}_{zyx, \text{PRF} \rightarrow \text{SRF}} \begin{bmatrix} x \\ y \\ z \end{bmatrix}_{\mathbf{q}_{\text{PRF}}} . \quad (278)$$

Since the spacecraft size with respect to the ground pixel size and geolocation knowledge requirements [RD4] is relatively small, translation is neglected here. The alignment measurements between the payload reference frame and the spacecraft reference frame, which are measured between the IAC (which is placed on the UVN module) and SAC (which is placed on the top floor of the satellite), yield a correction to the above defined rotation matrix, to result in

$$\mathbf{R}_{zyx, \text{PRF} \rightarrow \text{SRF}} = \begin{bmatrix} -0.9999996580 & -0.0005925940 & +0.0005759130 \\ +0.0008010310 & -0.8663391140 & +0.4994556011 \\ +0.0002029614 & +0.4994558919 & +0.8663392931 \end{bmatrix} . \quad (279)$$

If the payload and the satellite, which are connected by the telescope support structure (TSS), were perfectly solid, the above transformation would suffice. However, the UVN and SWIR module are placed separately on the TSS, which will deform due to temperature gradients. The TSS in its turn is attached to the top floor of the satellite, which will also deform due to temperature gradients and due to the acceleration and vibrations during launch. Multiple temperature sensors are attached to the TSS and the top floor to measure the temperature gradients in-flight. During calibration testing, one alignment cube will be placed on the SWIR module and one on the TSS, to test their alignment in different environments.

A static gravity release rotation matrix will be supplied to account for the deformations due to the launch. Furthermore, two temperature dependent rotation matrices will be set up to account for the in-flight deformations of the TSS and top floor due to temperature gradients. The elements in this matrix will thus be a function of the temperatures as measured by the temperature sensors. Finally, also relative movement of the SWIR module with respect to the UVN module (to which the OAC is attached) has to be accounted for, which will also be described by a rotation matrix.

26.2.2 Payload roll error correction

To correct for the error in roll of the payload due to thermal deformation of the top floor of the spacecraft, the temperature of the top floor is determined. Eight thermistors that are placed on the foots of the bi-pods (one on each foot of the small bi-pods and two on each foot of the large bi-pods), which connect the payload and TSS to the top floor, will measure temperature. Thermal analysis of the spacecraft shows that the average of these 8 temperature measurements is representative for the temperature of the top floor at any time t (accurate to ± 0.5 K, where the thermistor pairs on the large bi-pods are averaged beforehand, so the average is then taken over 6 temperatures,

$$T_{\text{topfloor}}(t) = \frac{1}{6} \left[\sum_{i=1}^4 T_{\text{th}_i}(t) + \frac{T_{\text{th}_5} + T_{\text{th}_6}}{2} + \frac{T_{\text{th}_7} + T_{\text{th}_8}}{2} \right] . \quad (280)$$

Over one orbit, this top floor temperature will have a maximum variation of 2 K. All N temperature measurements t_j in an orbit are averaged,

$$T_{\text{TForbit}} = \frac{1}{N} \sum_{j=1}^N T_{\text{topfloor}}(t_j) . \quad (281)$$

If a thermistor measures a temperature deviating more than 3 K from all other thermistors, it fails, and the neighboring bi-pod foot thermistor or neighboring thermistor on the same foot temperature measurement is used instead of the failed one.

The roll (across-track) error can be scaled with the difference between the top floor temperature in-orbit and during on-ground alignment,

$$\Delta_{\text{roll}} = k(T_{\text{TFalignment}} - T_{\text{TForbit}}) , \quad (282)$$

where the scaling factor k is a function of the thermal expansion coefficient of the top floor and of the geometry of the bi-pods, and the reference alignment temperature is 293.15 K. A preliminary value for this factor is

$k = 14.15 \mu\text{rad/K}$ for the coldest scenario (BOL, summer solstice), and $k = 11.75 \mu\text{rad/K}$ for the warmest scenario (EOL, winter solstice). If the on-orbit top-floor temperature is smaller than the alignment temperature, the roll angle will be positive. At the equator, this results in a ground pixel displacement westwards (i.e. the actual position of a pixel is further westward than is calculated using only the quaternion, which is described below).

26.2.3 Spacecraft reference frame to inertial reference frame

For the transformation of a point in the spacecraft reference frame to the inertial reference frame the attitude measurement of the STR system is used, which is defined as a unit quaternion from the inertial reference frame to the spacecraft reference frame

$$\mathbf{q} = \begin{bmatrix} q_x \\ q_y \\ q_z \\ q_s \end{bmatrix}, \quad (283)$$

with which the passive right-handed rotation matrix from the inertial reference frame (IRF) to the spacecraft reference frame (SRF) is defined as

$$\mathbf{R}_{\text{IRF} \rightarrow \text{SRF}} = \begin{bmatrix} 1 - 2(q_y^2 + q_z^2) & 2(q_x q_y + q_z q_s) & 2(q_x q_z - q_y q_s) \\ 2(q_x q_y - q_z q_s) & 1 - 2(q_x^2 + q_z^2) & 2(q_y q_z + q_x q_s) \\ 2(q_x q_z + q_y q_s) & 2(q_y q_z - q_x q_s) & 1 - 2(q_x^2 + q_y^2) \end{bmatrix}. \quad (284)$$

Using this matrix the transformation of a point \mathbf{q} between the spacecraft reference frame and the inertial reference frame is obtained by evaluating

$$\mathbf{R}_{\text{IRF} \rightarrow \text{SRF}}(\mathbf{q}_{\text{IRF}} - \mathbf{p}_{\text{IRF}}) = \mathbf{q}_{\text{SRF}}, \quad (285a)$$

$$\mathbf{q}_{\text{IRF}} = (\mathbf{R}_{\text{IRF} \rightarrow \text{SRF}})^{-1} \mathbf{q}_{\text{SRF}} + \mathbf{p}_{\text{IRF}} = (\mathbf{R}_{\text{IRF} \rightarrow \text{SRF}})^T \mathbf{q}_{\text{SRF}} + \mathbf{p}_{\text{IRF}}, \quad (285b)$$

as the rotation matrix is orthogonal and thus its inverse is equal to its transpose, and in which \mathbf{p}_{IRF} is the position of the spacecraft in the inertial reference frame to account for translation of the origin of the reference frame to the center of mass of the spacecraft.

To determine the intersection of a unit direction LOS vector extending from the known location of the spacecraft (reference frame) with the Earth reference ellipsoid in the Earth-fixed reference frame, only the rotation has to be applied. The equation for the LOS (and for direction vectors in general) therefore simplifies to

$$\hat{\mathbf{q}}_{\text{IRF}} = (\mathbf{R}_{\text{IRF} \rightarrow \text{SRF}})^T \hat{\mathbf{q}}_{\text{SRF}}. \quad (286)$$

26.2.4 Aberration of Light

Due to the finite speed of light and the motion of the spacecraft (reference frame) with respect to the Earth(-fixed reference frame), an apparent motion of the point observed on Earth occurs. This astrophysical phenomenon is called the aberration of light, and the deviation in LOS angle depends only on the transverse velocity of the spacecraft, with respect to the LOS. As the spacecraft moves with a large velocity with respect to the Earth relative to the speed of light (approx. 7.44/300000 km/s), this effect can amount up to 50 meters at the edge of swath, where the distance to the ground pixel is largest, while the velocity of the spacecraft is approximately orthogonal to the LOS.

This effect is corrected for as follows, and can be configured to be set on or off. When the LOS vector in the spacecraft reference frame \mathbf{q}_{SRF} is rotated to the inertial reference frame \mathbf{q}_{IRF} (hereafter denoted simply as $\mathbf{q} = (x, y, z)$), the vector is first normalized as

$$\hat{\mathbf{q}} = \frac{\mathbf{q}}{\|\mathbf{q}\|} = \frac{x}{\|\mathbf{q}\|} \hat{\mathbf{x}} + \frac{y}{\|\mathbf{q}\|} \hat{\mathbf{y}} + \frac{z}{\|\mathbf{q}\|} \hat{\mathbf{z}}, \quad (287)$$

in which $\|\mathbf{q}\|$ denotes the length of the vector \mathbf{q} defined as

$$\|\mathbf{q}\| = \sqrt{x^2 + y^2 + z^2}. \quad (288)$$

The velocity of the spacecraft in the inertial reference frame \mathbf{v} relative to the speed of light c is subtracted from this normalized vector as

$$[\hat{\mathbf{q}}]_{\text{abb}} = \hat{\mathbf{q}} - \frac{\mathbf{v}}{c}, \quad (289)$$

which is normalized again as

$$\hat{\mathbf{q}}_{\text{abb}} = \frac{[\hat{\mathbf{q}}]_{\text{abb}}}{\|[\hat{\mathbf{q}}]_{\text{abb}}\|}, \quad (290)$$

and then scaled back to the original length as

$$\mathbf{q}_{\text{abb}} = \|\mathbf{q}\| \hat{\mathbf{q}}_{\text{abb}}. \quad (291)$$

This resulting vector that is corrected for aberration of light can now be translated in the inertial reference frame, if needed. When the input vector in the spacecraft reference frame is already a unit vector, Equations (287) and (291) can be skipped.

A similar effect, called light-time, which occurs due to the rotation of the Earth during the time the light has travelled from the Earth to the spacecraft, amounts to a maximum of about 3 meters at the edge of swath, and is ignored here.

26.2.5 Inertial reference frame to Earth-fixed reference frame

The transformation of either a position or velocity vector from the inertial to the Earth-fixed reference frame, are described separately.

26.2.5.1 Position transformation The transformation between the inertial reference frame and the Earth-fixed reference frame, is rigorously documented in [RD14] (Chapter 5). However, in this reference document, the reference frames are called geocentric celestial reference system (GCRS) and international terrestrial reference system (ITRS), respectively.

The transformation is performed by multiplying the Cartesian coordinates in the inertial reference frame (IRF) with three rotation matrices, to obtain the coordinates in the Earth-fixed reference frame:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix}_{\text{EFRF}} = \mathbf{W}(t)\mathbf{R}(t)\mathbf{Q}(t) \begin{bmatrix} x \\ y \\ z \end{bmatrix}_{\text{IRF}}. \quad (292)$$

Here, $\mathbf{Q}(t)$, $\mathbf{R}(t)$ and $\mathbf{W}(t)$ are three transformation matrices, which are functions of TT and UT1 in JD, and are described below.

$\mathbf{Q}(t)$ arises from the motion of the celestial pole in the inertial reference frame. This motion consists of two superimposed motions, called precession and nutation. These are both shown schematically in Figure 57. Precession is a circular motion of the polar axis with an angular radius of about 23.4° , centered on the ecliptic North pole and directed West. Nutation is a relatively small sinusoidal motion superposed on precession. Both are mainly caused by the gravitational attraction of the Sun and the Moon, the gravitational effect of their changing relative positions, the excess of mass at the Earth's equator and, to a lesser extent, by other celestial bodies.

$\mathbf{R}(t)$ arises from the rotation of the Earth around the axis associated with the pole. The Earth rotates about its polar axis to the East, with a nominal angular velocity in inertial space of about $7.292 \cdot 10^{-5}$ rad/s, as indicated in Figure 57. The Earth rotates once in about 24 hours from the point of view of the Sun and once every 23 hours, 56 minutes and 4 seconds from the point of view of the stars. The Earth's rotation is slowing slightly with time. This is due to the tidal effects of the Moon on the Earth's rotation. Atomic clocks show that a modern day is longer by about 17 milliseconds than a century ago, slowly increasing the rate at which UTC is adjusted by leap seconds.

Finally, $\mathbf{W}(t)$ arises from polar motion. The polar motion of the Earth is the movement of the Earth's rotational axis across its surface, and is measured with respect to the Earth-fixed Reference Frame. The variation here is only a few meters. It consists of two quasi-periodic components and a gradual drift. This gradual drift is defined as the movement of the Earth's instantaneous rotational axis or North pole, from the CIO (Conventional International Origin), mostly in the direction of the 80th meridian west. The CIO is a conventionally agreed reference axis, defined as the pole's average location over the year 1900. The two periodic parts describe an almost circular motion called Chandler wobble, with a period of about 435 days, and a yearly circular motion, including a small drift. These motions are illustrated in Figure 58.

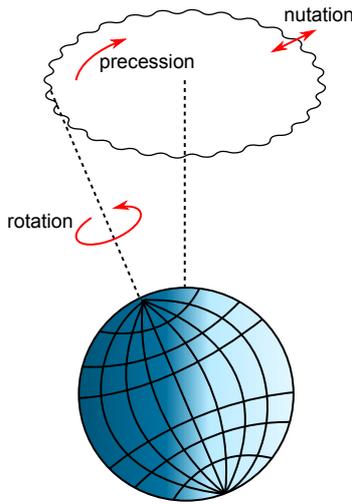


Figure 57: Schematic of two motions of the Earth's polar axis, precession and nutation, and the rotation about this axis.

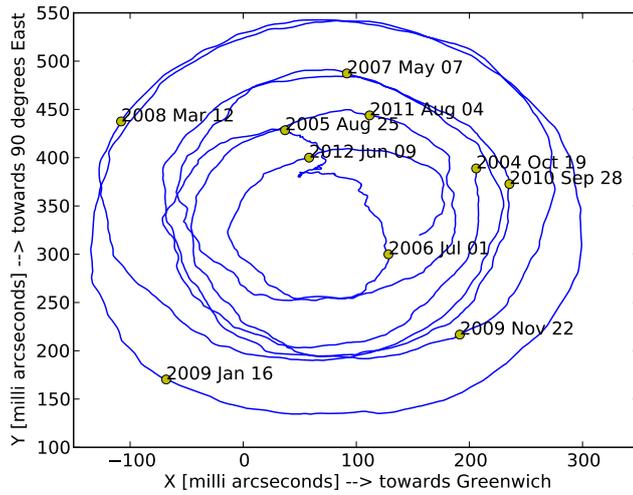


Figure 58: Plot of the polar coordinate x_p versus y_p .

The transformation expressed by Equation (292) can be performed in two ways, as described in [RD14]. The classical procedure realizes a “true equinox and equator of date system” at date t , that uses the Celestial Intermediate Pole (CIP) as its Z -axis and the equinox as its X -axis. It uses apparent Greenwich Sidereal Time (GST) in the transformation matrix $\mathbf{R}(t)$ and the classical precession and nutation parameters in the transformation matrix $\mathbf{Q}(t)$. The newer method realizes a “Celestial Intermediate Reference System” (CIRS) at date t . The CIRS uses the CIP as its Z -axis and the CIO as its X -axis. The “Earth Rotation Angle” is used in the transformation matrix $\mathbf{R}(t)$, and the two coordinates of the Celestial Intermediate Pole (CIP) in the GCRS in the transformation matrix $\mathbf{Q}(t)$. However, the last step, multiplying with the rotation matrix $\mathbf{W}(t)$ for polar motion, which transforms from the terrestrial intermediate reference system (TIRS) to the ITRS, is the same for both methods. The exact details of these implementations can be found in [RD14].

The required input is: the time instance for which the transformation matrix is needed, as Terrestrial Time (TT) and Universal Time (UT1), expressed in Julian Days, and the polar coordinates x_p and y_p . Monthly bulletin B, which is published by the IERS, contains daily values for these polar coordinates, along with the difference between UTC (which can be converted to TT using Equations (268) and (273)) and UT1. These values can then be interpolated to yield an approximation that holds for the time instance at hand.

The celestial motion of the CIP (precession-nutation), includes all the terms with periods greater than two days in the GCRS, i.e. frequencies between -0.5 cycles per sidereal day (cpsd) and +0.5 cpsd. The terrestrial motion of the CIP (polar motion), includes all the terms outside the retrograde diurnal band in the ITRS i.e. frequencies lower than -1.5 cpsd or greater than -0.5 cpsd.

26.2.5.2 Velocity transformation Differentiating the equation for the transformation of a position vector from the inertial to the Earth-fixed reference frame, yields

$$\frac{d\mathbf{p}_{\text{EFRF}}}{dt} = \frac{d[\mathbf{W}(t)\mathbf{R}(t)\mathbf{Q}(t)]}{dt} \mathbf{p}_{\text{IRF}} + [\mathbf{W}(t)\mathbf{R}(t)\mathbf{Q}(t)] \frac{d\mathbf{p}_{\text{IRF}}}{dt} \quad (293)$$

However, employing the conversion method involving the CIRS and TIRS using the CIO, this can be approximated stepwise as

$$\frac{d\mathbf{p}_{\text{CIRS}}}{dt} = \mathbf{Q}(t) \frac{d\mathbf{p}_{\text{IRF}}}{dt} \quad (294)$$

$$\frac{d\mathbf{p}_{\text{TIRS}}}{dt} = \mathbf{R}(t) \frac{d\mathbf{p}_{\text{CIRS}}}{dt} + \frac{d\mathbf{R}(t)}{dt} \mathbf{p}_{\text{CIRS}} \quad (295)$$

$$\frac{d\mathbf{p}_{\text{EFRF}}}{dt} = \mathbf{W}(t) \frac{d\mathbf{p}_{\text{TIRS}}}{dt}, \quad (296)$$

in which the time rate of change of $\mathbf{W}(t)$ and $\mathbf{Q}(t)$ are assumed to be negligably small. For an analogous derivation using the classical method involving precession/nutation and GST, see the Appendix of [RD15].

This results in

$$\frac{d\mathbf{p}_{\text{EFRF}}}{dt} = \mathbf{W}(t) \left[\mathbf{R}(t)\mathbf{Q}(t) \frac{d\mathbf{p}_{\text{IRF}}}{dt} + \frac{d\mathbf{R}(t)}{dt} \mathbf{Q}(t) \mathbf{p}_{\text{IRF}} \right], \quad (297)$$

in which the rotation about the CIP is defined as

$$\mathbf{R}(t) = \begin{bmatrix} +\sin \theta & +\cos \theta & 0 \\ -\cos \theta & +\sin \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (298)$$

in which θ is the Earth Rotation Angle (ERA).

The time rate of change of this rotation matrix is evaluated as

$$\frac{d\mathbf{R}(t)}{dt} = \begin{bmatrix} -\dot{\theta} \sin \theta & +\dot{\theta} \cos \theta & 0 \\ -\dot{\theta} \cos \theta & -\dot{\theta} \sin \theta & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (299)$$

in which the rate of advance of ERA is given in [RD14] as

$$\dot{\theta} = 1.00273781191135448 \text{ rev/day}_{\text{UT1}}, \quad (300)$$

which can be converted as

$$\dot{\theta} = \frac{1.00273781191135448 * 2 * \pi}{86400 + \text{LOD}} \text{ rad/s}, \quad (301)$$

in which The Length of Day (LOD) is the difference between a day as measured by UT1 and a 86400 seconds SI day, which is supplied in the IERS Bulletin B file.

26.2.6 Geocentric to geodetic coordinates

As follows from Figures 50 and 52, the conversion from geocentric (c) spherical to geocentric (c) Cartesian coordinates is given by

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix}_c = r \begin{bmatrix} \cos \delta' \cos \vartheta \\ \cos \delta' \sin \vartheta \\ \sin \delta' \end{bmatrix}_c, \quad (302)$$

while conversion from geodetic (d) to geocentric (c) Cartesian coordinates is given by

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix}_c = \begin{bmatrix} (N_\delta + h) \cos \delta \cos \vartheta \\ (N_\delta + h) \cos \delta \sin \vartheta \\ ((1 - e^2)N_\delta + h) \sin \delta \end{bmatrix}_d, \quad (303)$$

where e is the eccentricity of the ellipsoid

$$e \equiv \frac{\sqrt{a^2 - b^2}}{a} = \sqrt{2f - f^2} \quad (304)$$

and N_δ is the ellipsoidal radius of curvature in the meridian, given by

$$N_\delta \equiv \frac{a}{\sqrt{1 - e^2 \sin^2 \delta}}. \quad (305)$$

Conversion from geocentric Cartesian to geocentric spherical coordinates is given by

$$\begin{bmatrix} \delta' \\ \vartheta \\ r \end{bmatrix}_c = \begin{bmatrix} \arctan \left(\frac{z}{\sqrt{x^2 + y^2}} \right) \\ \arctan 2(y, x) \\ \sqrt{x^2 + y^2 + z^2} \end{bmatrix}_c, \quad (306)$$

where $\delta' = \arcsin(z/r)$ can also be used, and $\arctan2$ ensures ϑ is evaluated as $-\pi < \vartheta \leq \pi$.

However, a solution for the conversion from geocentric Cartesian to geodetic coordinates is not that simple, as has been documented in many references. The conversion is performed here with the fastest available method up to date, as described in [RD16]. With this method the WGS84 Earth reference ellipsoid is set as the reference ellipsoid for which the conversion is performed.

26.2.7 Earth-fixed reference frame to topocentric reference frame

The rotation matrix from the geocentric Cartesian coordinates in the Earth-fixed reference frame to the topocentric reference frame depends only on the longitude ϑ and geodetic latitude δ , and is derived as

$$\mathbf{R}_{\text{EFRF} \rightarrow \text{TRF}} = \begin{bmatrix} -\sin \vartheta & \cos \vartheta & 0 \\ -\sin \delta \cos \vartheta & -\sin \delta \sin \vartheta & \cos \delta \\ \cos \delta \cos \vartheta & \cos \delta \sin \vartheta & \sin \delta \end{bmatrix}. \quad (307)$$

And so a transformation of a point \mathbf{q} is performed as

$$\mathbf{q}_{\text{TRF}} = \mathbf{R}_{\text{EFRF} \rightarrow \text{TRF}}(\mathbf{q}_{\text{EFRF}} - \mathbf{r}_{\text{EFRF}}), \quad (308)$$

in which \mathbf{r}_{EFRF} is the radius vector of the origin of the topocentric reference frame, which is obtained by using $h = 0$ in Equation (303), to account for the translation of the origin of this frame.

26.2.8 Inertial reference frame to local orbital reference frame

Since the local orbital reference frame is defined by the position $\mathbf{p} = [x, y, z]$ and velocity $\mathbf{v} = [\dot{x}, \dot{y}, \dot{z}]$ of the spacecraft in the inertial reference frame, the rotation matrix from the inertial reference frame (X, Y, Z) , with unit vectors $(\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}})$, to the local orbital reference frame (T, R, L) , with unit vectors $(\hat{\mathbf{t}}, \hat{\mathbf{r}}, \hat{\mathbf{l}})$, can be based upon this state-vector only. To this end the measured state-vector by the GNSS in the Earth-fixed reference frame has to be transformed to the inertial reference frame first, as described in Section 26.2.5. Following the definition of the local orbital reference frame from Section 26.1.7, the position vector \mathbf{p} points in the direction of the L -axis, and thus the unit vector $\hat{\mathbf{l}}$ of that axis is obtained by normalizing \mathbf{p}

$$\hat{\mathbf{l}} = \hat{\mathbf{p}} = \frac{\mathbf{p}}{\|\mathbf{p}\|} = \frac{x}{\|\mathbf{p}\|} \hat{\mathbf{x}} + \frac{y}{\|\mathbf{p}\|} \hat{\mathbf{y}} + \frac{z}{\|\mathbf{p}\|} \hat{\mathbf{z}}, \quad (309)$$

in which $\|\mathbf{p}\|$ denotes the length of the vector \mathbf{p} defined as

$$\|\mathbf{p}\| = \sqrt{x^2 + y^2 + z^2}. \quad (310)$$

Then, since the velocity vector \mathbf{v} does lie in the orbital plane but is not necessarily directed along the R -axis, the component of \mathbf{v} in the direction of $\hat{\mathbf{l}}$ is first determined by using the geometrical inner product rule, and using $\|\hat{\mathbf{l}}\| = 1$, as

$$v_{\hat{\mathbf{l}}} = \frac{(\mathbf{v}, \hat{\mathbf{l}})}{\|\hat{\mathbf{l}}\|} = \mathbf{v}^T \hat{\mathbf{l}} = \frac{x\dot{x}}{\|\mathbf{p}\|} + \frac{y\dot{y}}{\|\mathbf{p}\|} + \frac{z\dot{z}}{\|\mathbf{p}\|}, \quad (311)$$

which is subtracted from \mathbf{v} to yield the component of \mathbf{v} in the direction of $\hat{\mathbf{r}}$ as

$$\mathbf{v}_{\hat{\mathbf{r}}} = \mathbf{v} - v_{\hat{\mathbf{l}}} \hat{\mathbf{l}}, \quad (312)$$

which is normalized to yield the unit vector $\hat{\mathbf{r}}$ of the R -axis as

$$\hat{\mathbf{r}} = \frac{\mathbf{v}_{\hat{\mathbf{r}}}}{\|\mathbf{v}_{\hat{\mathbf{r}}}\|}. \quad (313)$$

Then, the unit vector $\hat{\mathbf{t}}$ of the T -axis is derived by taking the cross product of $\hat{\mathbf{r}}$ and $\hat{\mathbf{l}}$

$$\hat{\mathbf{t}} = \hat{\mathbf{r}} \times \hat{\mathbf{l}}. \quad (314)$$

Equation (309) is used for $\hat{\mathbf{l}}$. Equation (311) is substituted in Equation (312), and the result in Equation (313) to get an expression for $\hat{\mathbf{r}}$. Then, the resulting expressions for $\hat{\mathbf{l}}$ and $\hat{\mathbf{r}}$ are substituted in Equation (314) to yield equations for the unit vectors which we denote now in the form

$$\hat{\mathbf{t}} = \hat{t}_x \hat{\mathbf{x}} + \hat{t}_y \hat{\mathbf{y}} + \hat{t}_z \hat{\mathbf{z}}, \quad (315a)$$

$$\hat{\mathbf{r}} = \hat{r}_x \hat{\mathbf{x}} + \hat{r}_y \hat{\mathbf{y}} + \hat{r}_z \hat{\mathbf{z}}, \quad (315b)$$

$$\hat{\mathbf{l}} = \hat{l}_x \hat{\mathbf{x}} + \hat{l}_y \hat{\mathbf{y}} + \hat{l}_z \hat{\mathbf{z}}, \quad (315c)$$

in which the components are all evaluated as functions of (x, y, z) and $(\dot{x}, \dot{y}, \dot{z})$. These components are then inserted in the rotation matrix $\mathbf{R}_{\text{IRF} \rightarrow \text{LORF}}$ as

$$\mathbf{R}_{\text{IRF} \rightarrow \text{LORF}} = \begin{bmatrix} \hat{\mathbf{t}}^T \\ \hat{\mathbf{r}}^T \\ \hat{\mathbf{l}}^T \end{bmatrix} = \begin{bmatrix} \hat{t}_x & \hat{t}_y & \hat{t}_z \\ \hat{r}_x & \hat{r}_y & \hat{r}_z \\ \hat{l}_x & \hat{l}_y & \hat{l}_z \end{bmatrix}, \quad (316)$$

which is used to transform any point \mathbf{q} in the inertial reference frame to a point in the local orbital reference frame as

$$\mathbf{q}_{\text{LORF}} = \mathbf{R}_{\text{IRF} \rightarrow \text{LORF}}(\mathbf{q}_{\text{IRF}} - \mathbf{p}_{\text{IRF}}), \quad (317)$$

in which also the translation of the origin of the reference frame to the center of mass of the spacecraft is included.

26.2.9 Payload reference frame to Sun port reference frame

The transformation from the payload reference frame (Section 26.1.10) to the Sun port reference frame (Section 26.1.12) is needed to determine the LOS from the spacecraft towards the Sun with respect to the Sun port. As the dimensions of the spacecraft are negligible with respect to the distance towards the Sun, translations are neglected here, and so only a rotation is needed for the transformation. The rotation matrix from the payload reference frame to the Sun port reference frame is evaluated as

$$\mathbf{R}_{\text{PRF} \rightarrow \text{SPRF}} = \mathbf{R}_{xy'z''} \left(\frac{\pi}{2}, -\frac{\pi}{2} + \text{AZO}, \frac{\pi}{2} \right) = \begin{bmatrix} 0 & 0 & 1 \\ -\cos\left(-\frac{\pi}{2} + \text{AZO}\right) & -\sin\left(-\frac{\pi}{2} + \text{AZO}\right) & 0 \\ +\sin\left(-\frac{\pi}{2} + \text{AZO}\right) & -\cos\left(-\frac{\pi}{2} + \text{AZO}\right) & 0 \end{bmatrix}, \quad (318)$$

in which AZO is the azimuth offset angle, which is the angle between the normal of the inner Sun baffle vane and the Z-axis of the Sun port reference frame. The transformation of a point $\mathbf{q} = [x, y, z]$ from the payload reference frame to the Sun port reference frame can then be evaluated as

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix}_{\mathbf{q}_{\text{SPRF}}} = \mathbf{R}_{\text{PRF} \rightarrow \text{SPRF}} \begin{bmatrix} x \\ y \\ z \end{bmatrix}_{\mathbf{q}_{\text{PRF}}}. \quad (319)$$

Although this definition does not exactly match with, for instance, the normal to the Sun port baffle, due to mechanical imprecision, it is chosen as the implemented conversion between the two frames. Alignment measurements are used for the relevant on-ground measurements.

26.2.10 Earth-fixed reference frame to Fundamental reference frame

The rotation from the geocentric Cartesian coordinates in the Earth-fixed reference frame to the (solar eclipse) fundamental reference frame (see Section 26.1.14) depends only on the Greenwich Hour Angle μ and the geocentric equatorial declination angle d of the Z-axis of the Fundamental reference frame, and is given in [RD17] as

$$\rho_{\text{F}} = \mathbf{R}_1 \left(\frac{\pi}{2} - d \right) \mathbf{R}_3 \left(- \left(\mu - \frac{\pi}{2} \right) \right) \rho_{\text{G}} \quad (320)$$

from which the following rotation matrix is derived

$$\mathbf{R}_{\text{EFRF} \rightarrow \text{FRF}} = \begin{bmatrix} \sin \mu & \cos \mu & 0 \\ -\sin d \cos \mu & \sin d \sin \mu & \cos d \\ \cos d \cos \mu & -\cos d \sin \mu & \sin d \end{bmatrix}. \quad (321)$$

And so a transformation of a point \mathbf{q} is performed as

$$\mathbf{q}_{\text{FRF}} = \mathbf{R}_{\text{EFRF} \rightarrow \text{FRF}} \mathbf{q}_{\text{EFRF}}, \quad (322)$$

as the origins of both frames coincide.

26.3 Intersection between a line and an ellipsoid

Now follows an analysis on the intersection points of any line in 3-dimensional space and an ellipsoid that is attached to a reference frame. The equation of an ellipsoid centered at the origin of an Cartesian orthogonal coordinate system (X, Y, Z) , and with axis extents (e_x, e_y, e_z) in the direction of the (X, Y, Z) axes, respectively, is

$$\frac{x^2}{e_x^2} + \frac{y^2}{e_y^2} + \frac{z^2}{e_z^2} = 1. \quad (323)$$

The equation for a point \mathbf{p} on a line in this coordinate system is

$$\mathbf{p} = \mathbf{p}_0 + t\mathbf{v}, \quad (324)$$

or, expanded:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} + t \begin{bmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{bmatrix}, \quad (325)$$

in which $\mathbf{p}_0 = [x_0, y_0, z_0]$ is an initial point and $\mathbf{v} = [\dot{x}, \dot{y}, \dot{z}]$ is a constant (direction) vector. Set up a convenient matrix \mathbf{M} as

$$\mathbf{M} = \begin{bmatrix} e_x^{-2} & 0 & 0 \\ 0 & e_y^{-2} & 0 \\ 0 & 0 & e_z^{-2} \end{bmatrix}, \quad (326)$$

so we can write for the ellipsoid equation

$$\mathbf{p}^T \mathbf{M} \mathbf{p} = 1. \quad (327)$$

Substituting the equation for the line yields a quadratic equation

$$(\mathbf{p}_0 + t\mathbf{v})^T \mathbf{M} (\mathbf{p}_0 + t\mathbf{v}) = 1, \quad (328a)$$

$$(\mathbf{v}^T \mathbf{M} \mathbf{v})t^2 + (2\mathbf{p}_0^T \mathbf{M} \mathbf{v})t + (\mathbf{p}_0^T \mathbf{M} \mathbf{p}_0 - 1) = 0, \quad (328b)$$

that can be solved for two constants t_1 and t_2 with the quadratic formula as

$$t_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \quad (329)$$

with the coefficients (a, b, c) as

$$a = \mathbf{v}^T \mathbf{M} \mathbf{v} = \frac{\dot{x}^2}{e_x^2} + \frac{\dot{y}^2}{e_y^2} + \frac{\dot{z}^2}{e_z^2}, \quad (330a)$$

$$b = 2\mathbf{p}_0^T \mathbf{M} \mathbf{v} = 2 \left(\frac{x_0 \dot{x}}{e_x^2} + \frac{y_0 \dot{y}}{e_y^2} + \frac{z_0 \dot{z}}{e_z^2} \right), \quad (330b)$$

$$c = \mathbf{p}_0^T \mathbf{M} \mathbf{p}_0 - 1 = \frac{x_0^2}{e_x^2} + \frac{y_0^2}{e_y^2} + \frac{z_0^2}{e_z^2} - 1. \quad (330c)$$

Now there are three possibilities:

1. When the quadratic equation yields two distinct real roots for t_1, t_2 , the line intersects the ellipsoid, and these solutions yield two intersection points.
2. When there is only one real solution, the line is tangent to the ellipsoid, and this solution yields the only 'intersection' point.
3. When there are only complex solutions, the line does not intersect the ellipsoid, and there are no intersection points.

Filling in the value(s) for t in Equation (324) and (325) yields the intersection point(s). For the TROPOMI situation, the LOS extending from the spacecraft will hit the Earth on the front side first. So, the smallest absolute value for t is the intersection we are looking for, as the second intersection, with the largest absolute value for t , occurs at the backside of the Earth, as seen from the spacecraft. Furthermore, using the theory

above, intersections also occur for lines extending from the spacecraft in a direction opposite to that of the Earth. The intersection will then happen at negative values for t , as the 3D line will have a direction away from the Earth, but the mathematical description of this line will extend backwards too. One solution for t being positive while the other is negative is not possible here, as the spacecraft would have to reside within the Earth! So, the way to go about this intersection determining for TROPOMI is as follows:

- When possibility #3 occurs (i.e. the determinant $D = b^2 - 4ac < 0$), the LOS misses the Earth.
- When possibility #1 occurs (i.e. the determinant $D = b^2 - 4ac > 0$), and both solutions for t are negative, the LOS misses the Earth.
- When possibility #1 occurs (i.e. the determinant $D = b^2 - 4ac > 0$), and both solutions for t are positive, only the smallest solutions for t is used as the intersection of the LOS with the Earth.
- When possibility #2 occurs (i.e. the determinant $D = b^2 - 4ac = 0$), and the only solutions for t is negative, the LOS misses the Earth.
- When possibility #2 occurs (i.e. the determinant $D = b^2 - 4ac = 0$), and the only solutions for t is positive, this solution is used as the 'intersection' of the LOS with the Earth.

26.4 Instrument viewing definitions

In order to answer the question: "Where does the detected signal come from?", a thorough understanding of the viewing properties of the instrument is needed. This question is not trivial to answer due to the fact that TROPOMI data are acquired under dynamic conditions, i.e., with the instrument orbiting the Earth. In addition, TROPOMI is a hyperspectral imager, using an along track scanning method to build up the desired three-dimensional data cube that spans the wavelength, latitude and longitude dimensions. In order to annotate a measured TROPOMI datum with the geo-spatial origin of the detected radiation, the *optical transfer function* concept needs to be introduced. In the subsequent paragraphs we will use a heuristic derivation to arrive at the functions and definitions that are needed to understand the instrument's optical behavior. We will start with a description of the instrument's viewing properties under static conditions by ignoring the motion of the instrument as well as the time integration used during signal detection. Most terms and definitions, e.g. object and image space, are similar to those used for simple camera systems, but are extended and generalized such to make them suitable for hyperspectral imagers under dynamic conditions.

26.4.1 TROPOMI functional spaces

Firstly, we need to define the various functional *spaces* that exist for the TROPOMI observing system. The observing system aims at collecting back-scattered sunlight from the Earth's surface and atmosphere on a discrete geo-spatial grid. Geographical gridded data is commonly expressed using ground pixels on a representation of this surface. We here define the **Earth space** as the curved surface of the Earth, described by the WGS84 reference ellipsoid using the geodetic Earth fixed coordinate system (see Figure 52). Note that this space is not a flat plane but rather a curved one, and that is unambiguously described using the longitude and latitude coordinates.

The **detector space** is defined as the space that is spanned by the physical detection system. For TROPOMI the physical detection system consist of two-dimensional rectangular arrays of individual sensors (detector pixels) in a regular grid. These sensor arrays are placed in the focal plane of the instrument and referred to as the *focal plane array* or *detector*. This space is uniquely described using the dimensions row and column $[r_{\text{det}}, c_{\text{det}}]$. Note that these dimensions do not necessarily coincide with other dimensions in other spaces due to alignment errors and optical aberrations.

The aforementioned Earth space is projected onto the detector space by the TROPOMI instrument and this projection is the transformation we are looking for. In order to determine this transformation we now have to describe the optical properties of the instrument itself. To do this, the Earth and detector spaces are not practical. This is solved by introducing the object and image spaces:

The **object space** of TROPOMI is the space that is projected by the optical system onto the detection system's focal plane. This space is described by a set of spherical coordinates in the payload reference frame of which the radius coordinate is ignored, and to which a wavelength dimension is added. For TROPOMI the object coordinates thus are azimuth angle, elevation angle and wavelength $(\phi, \varepsilon, \lambda)$. Polarization is ignored here for simplicity, and the origin of this space is on the instrument alignment cube. The bottom-right plot in

Figure 54 shows the important details of this reference frame. The object space elevation angle is measured positive from nadir direction (the Z-axis in the payload reference frame) towards flight direction (the X-axis in the payload reference frame). The object space azimuth angle is measured positive from nadir direction (the Z-axis in the payload reference frame) towards the right-handed perpendicular axis (the Y-axis in the payload reference frame) with respect to the flight direction (the X-axis in the payload reference frame).

The **image space** is the focal plane of the optical system. This space is described by geometric coordinates $[X, Y]$, in which X is in the spectrometer wavelength dispersion direction, and Y perpendicular to the X -dimension. Its origin is arbitrarily chosen somewhere in the focal plane. In the projection of the TROPOMI object space onto the image space one dimension is apparently lost: the azimuth direction maps onto the focal plane Y direction, but the elevation direction coincides with the spectral dispersion in the X dimension, and thus seems to disappear. The wavelength dimension occupies the focal plane X dimension, and this is the crucial complication of a hyperspectral system as compared to an ordinary camera system. Thus, definitions used for simple camera systems must be extended in order to fully understand the mapping from three dimensions onto two dimensions.

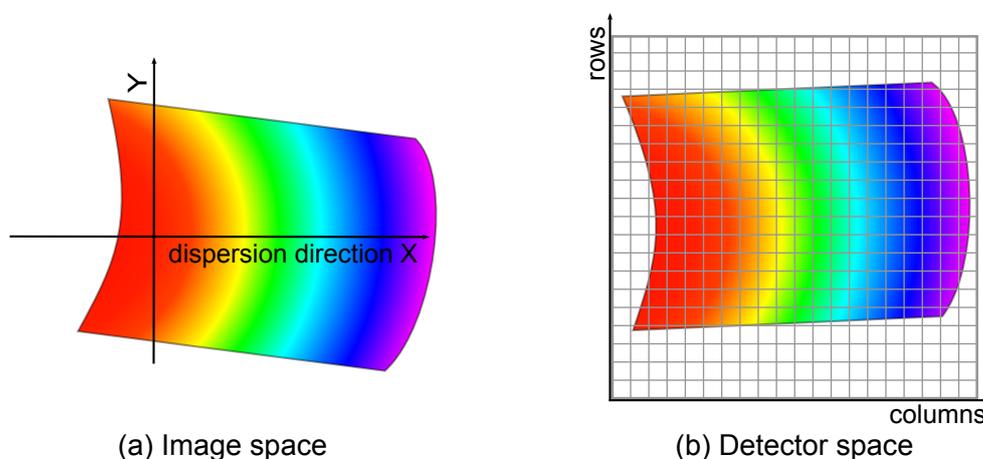


Figure 59: Illustration of the image space and the detector space. Note that the column dimension is not necessarily identical with the dispersion direction but can be tilted. The “smile” of the instrument prevents that the wavelength is constant over all rows in one column.

26.4.2 The general transfer function

A helpful general concept to understand the mapping between unequal dimensions is the **instrument transfer function**, also known in other disciplines as the system function or network function. This is a mathematical representation – in terms of spatial or temporal frequency – of the relation between the input and output of a linear time-invariant system with zero initial conditions and zero-point equilibrium. For optical imaging systems (under time invariant, i.e. static illumination conditions), the instrument transfer function is the Fourier transform of a generalized point source, and thus the mathematical description of the projection of the object space onto the image space. For TROPOMI this transformation is described by the projection of the three-dimensional space $(\phi, \epsilon, \lambda)$ onto the two-dimensional space $[X, Y]$. The instrument transfer function of an optical imaging system is also referred to as the **optical transfer function**. The **modulation transfer function** is the magnitude component of this (complex) optical transfer function.

26.4.3 Spread and response

Let us now introduce the notion of spread and response: the term **spread** denotes the projection of the object space onto the image space. Under practical conditions this projection is a one-to-many relationship; due to physical limitations a single point in object space will be blurred and reach multiple points in image space. The term **response** denotes the projection of the image space onto the object space. Under practical conditions this projection is a many-to-one relationship; due to physical limitations multiple separate points in object space will contribute to a single point in image space. See Figure 60 for a graphical presentation.

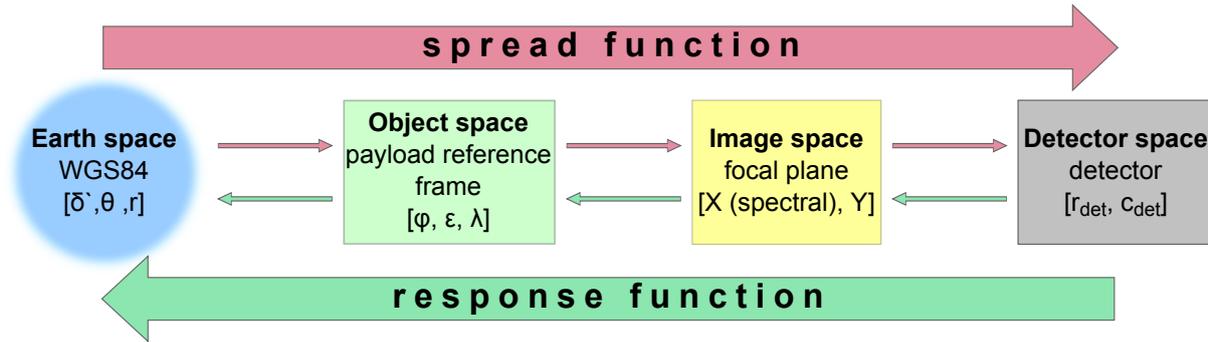


Figure 60: The transformation between object space and image space as described by the spread and response optical transfer functions.

26.4.4 Point source and point spread function

Some clarification of the term point source is needed here: In geometrical optics a **point source** is a true geometric point, with dimensions zero by zero. In practice, the actual source does not have to be infinitesimally small, but sufficiently small. A light source that can be treated mathematically as a point source for a specific optical system has an opening angle (divergence) which is smaller than the (spatial) resolution of the respective optical system. The spatial extent and the exact distance of the light source to the instrument can then be neglected. A point source can for example be a light source radiating in all directions placed at infinity or it can be a collimated source at a finite distance from the optical system. In case the optical system also has spectral resolving power, a monochromatic point source with a spectral width that is smaller than the spectral resolution of the optical system is used to determine the monochromatic point spread function.

Now we can define the **point spread function** as the irradiance distribution in the image space of a point source in object space. The point spread function determines the minimal spot size in the image space (focal plane) of an optical system. The minimal spot size is a measure for the resolution of the optical system. Due to the hyperspectral nature of TROPOMI, the generalized point spread function depends on all three object space dimension azimuth, elevation and wavelength (ϕ, ϵ, λ).

We can drop the wavelength dimension by writing down the expression for a single wavelength: The **monochromatic point spread function** is the irradiance distribution in the image space of a *monochromatic* point source. In other words, the monochromatic point spread function is the impulse reaction of an optical system at a single wavelength. For TROPOMI, the monochromatic point spread function at a specific wavelength depends only on the azimuth and elevation angle and it maps directly to a contiguous area in the image space.

26.4.5 Instrument response functions

The previous definitions describe the spread of a point source when looking into the instrument, i.e. from object space to image space. The instrument response function addresses the reverse transformation from image space onto object space, and can be thought of as looking out of the instrument: The **instrument response function** $\Psi_{\text{irf}}[X, Y]$ describes the response at each image space coordinate as a function of the object space dimensions (ϕ, ϵ, λ). The **instrument spectral response function** Ψ_{isrf} – also known as the slit function – is defined at each image space coordinate $[X, Y]$ and is solely a function of wavelength λ . The instrument spectral response function is the wavelength-dependent response of a focal plane point, and is equivalent to the instrument response function integrated over azimuth angle (ϕ) and elevation angle (ϵ):

$$\Psi_{\text{isrf}}[X, Y](\lambda) = \int \int \Psi_{\text{irf}}[X, Y] d\phi d\epsilon . \quad (331)$$

26.4.6 Pixel response functions

The aforementioned transfer function definitions are valid in the absence of a way to detect the signal in the focal plane. In practice a two-dimensional array of pixels (the detector) will be placed in the focal plane of the optical system to sample the image space onto a quantized grid. Thus, a conversion is made from image space coordinates to detector space coordinates, which includes a certain amount of integration of the response over the physical size of the pixel. We will now define the response functions in detector space for individual pixels of the detector array. The **pixel response function** $\Psi_{\text{prf}}[r_{\text{det}}, c_{\text{det}}]$ describes the relative

response of a single detector pixel $[r_{\text{det}}, c_{\text{det}}]$ as a function of the object space dimensions $(\phi, \varepsilon, \lambda)$. This base definition can be experimentally determined by registering the pixel response of a (monochromatic) point source sampling all prevailing wavelengths and azimuth and elevation angles. For each pixel individually, and at each wavelength, we can now define the **monochromatic line of sight** as the barycenter of the pixel response function, expressed as an azimuth and elevation angle pair in object space.

However, the interpretation using three dimensions is cumbersome, and it is convenient to define the following cross-sections of the pixel response function. The **monochromatic elevation response function** Ψ_{pmerf} of a detector pixel $[r_{\text{det}}, c_{\text{det}}]$ is the integral of the pixel response function over the azimuth angles (ϕ) at a single wavelength (λ) :

$$\Psi_{\text{pmerf}}[r_{\text{det}}, c_{\text{det}}](\lambda, \varepsilon) = \int \Psi_{\text{prf}}[r_{\text{det}}, c_{\text{det}}] d\phi . \quad (332)$$

The **monochromatic azimuth response function** Ψ_{pmarf} of a detector pixel $[r_{\text{det}}, c_{\text{det}}]$ is the integral of the pixel response function over the elevation angles (ε) for a single wavelength λ :

$$\Psi_{\text{pmarf}}[r_{\text{det}}, c_{\text{det}}](\lambda, \phi) = \int \Psi_{\text{prf}}[r_{\text{det}}, c_{\text{det}}] d\varepsilon . \quad (333)$$

The **pixel spectral response function** Ψ_{psrf} is defined per detector pixel $[r_{\text{det}}, c_{\text{det}}]$ and is solely a function of wavelength λ . This pixel spectral response function is the wavelength-dependent response of a detector pixel $[r_{\text{det}}, c_{\text{det}}]$ and is equivalent to the pixel response function integrated over azimuth angle (ϕ) and elevation angle (ε) :

$$\Psi_{\text{psrf}}[r_{\text{det}}, c_{\text{det}}](\lambda) = \int \int \Psi_{\text{prf}}[r_{\text{det}}, c_{\text{det}}] d\phi d\varepsilon . \quad (334)$$

The **pixel wavelength position** is now defined as the wavelength of the barycenter of the pixel spectral response function. Let us now take into account that a single detector pixel is sensitive to multiple wavelengths. The **pixel polychromatic spatial response function** Ψ_{pprf} is the angular sensitivity of each detector pixel $[r_{\text{det}}, c_{\text{det}}]$ as a function of elevation angle (ε) and azimuth angle (ϕ) integrated over all relevant wavelengths:

$$\Psi_{\text{pprf}}[r_{\text{det}}, c_{\text{det}}](\phi, \varepsilon) = \int \Psi_{\text{prf}}[r_{\text{det}}, c_{\text{det}}] d\lambda . \quad (335)$$

For TROPOMI this polychromatic response function is a two-dimensional surface whose axes are the object space azimuth and elevation angles. This is the actual quantity of importance that will be characterized during the on-ground calibration effort by using a white light point source (a so-called star stimulus) to sample all prevailing azimuth and elevation angles and recording all individual pixel responses.

In TROPOMI, individual detector pixels $[r_{\text{det}}, c_{\text{det}}]$ may be combined into an image pixel $[r_{\text{img}}, c_{\text{img}}]$ (where $c_{\text{img}} = c_{\text{det}}$) using a process known as row binning, which takes place on detector level. This binning process results in a **binned pixel response function** Ψ_{bprf} that is merely the direct sum of the individual pixel response functions weighted with their corresponding PRNU:

$$\Psi_{\text{bprf}}[r_{\text{img}}, c_{\text{img}}](\phi, \varepsilon) = \sum_{r_{\text{det}}=r_1}^{r_n} \Psi_{\text{prf}}[r_{\text{det}}, c_{\text{img}}](\phi, \varepsilon) \cdot c_{\text{prnu}}[r_{\text{det}}, c_{\text{img}}] , \quad (336)$$

where r_1 and r_n are the first and last detector rows that make up image row r_{img} . We have now described the required transformations between object, image and detector space. The final step is to describe the transformation from the object space to the Earth space. This transformation must include the motion of the instrument and is thus not time invariant.

26.4.7 Dynamically combined response functions

In general, a *measurement frame* of TROPOMI will consist of a two-dimensional array of binned detector pixels spanning the spatial and spectral dimensions that has been acquired during a single exposure time. In addition, multiple frames may be co-added over time (and thus added over the along-track spatial dimension) into a TROPOMI *measurement*. Here, we will skip the description of the monochromatic situation and directly continue with the polychromatic case as this is closest to the actual characterization approach. To obtain the **measurement polychromatic spatial response function** one must combine the polychromatic pixel response functions of all individual detector pixels involved in the measurement. This combination can include multiple instrumental effects:

- In the case of cross-track binning the measurement polychromatic spatial response function is the superposition of the individual polychromatic spatial response functions of the pixels involved in the binning process. Note that this superposition is weighted with the pixel response non-uniformity.
- For non-static conditions the polychromatic spatial response function is the convolution of the static polychromatic spatial response function over the integration time.
- In the case of temporal co-addition the polychromatic spatial response function is the superposition of the aforementioned convolved polychromatic spatial response functions.

The measurement polychromatic spatial response function is a function of azimuth and elevation angle (ϕ, ε) in object space and defined in image space for each set of binned detector rows in a column $[r_{\text{det}}, c_{\text{det}}]$ (with $r_{\text{det}} = r_1 \dots r_n$) that are involved in the measurement. The measurement polychromatic spatial response function is valid for a specific exposure time / co-addition period combination.

26.4.8 Line of sight

The line of sight of a single detector pixel $[r_{\text{det}}, c_{\text{det}}]$ is in the direction of the barycenter of the pixel polychromatic spatial response function for that pixel, given in the instrument reference frame, with the instrument alignment cube as the origin. The line of sight of a measurement is in the direction of the barycenter of the measurement polychromatic spatial response function, expressed in the corresponding object space coordinates (ϕ, ε) . This latter definition now includes all instrument effects that apply to TROPOMI: co-addition, cross-track binning, and optical artifacts like chromatic aberrations and spectral and spatial smiles of the imaging system. All these facts have to be taken into account in order to annotate a measurement (a set of binned and co-added detector pixels) in the spectral and geolocation domains. Note that this measurement line of sight is given in object space coordinates (ϕ, ε) ; these can be readily converted to Earth space coordinates using the algorithms in Section 27 to yield the **measurement ground pixel center coordinates**.

26.4.9 Ground pixel extent

In order to come to a definition of the **extent** of a ground pixel, an arbitrary choice has to be made on how to interpret the two-dimensional measurement polychromatic spatial response function. This can be done using integrated energy, full width at half maximum, halfway between two adjacent center coordinates, or any other metric that is considered appropriate by the Level-1b product user; see section 26.4.10 for a theoretical elaboration. It should be noted that for TROPOMI a cross-track ground position spectrum is assumed to be described by a row of (binned) pixels on the detector. It is not guaranteed that all pixels on such a row have exactly the same relative spatial response function and thus the same line of sight. This choice leads to the fact that spectral detector pixels in a row most likely do not observe exactly the same ground area. This effect is quantified using the concept of **co-registration**, which is defined as the amount of overlap between the measurement polychromatic spatial response function of all detector pixels in a row.

26.4.10 Formal computation of the ground pixel extent

We now proceed with a formal derivation of the polychromatic spatial response function. The adjective 'polychromatic' implies that we generalize in the spectral dimension: the related calibration measurements use a white light source star stimulus. In this way, an entire row of the detector is illuminated.

1. We start with the lines of sight of a single detector pixel. The LOS is defined as the two-tuple $(\varphi_M[\mathbf{x}_{\text{det}}], \varepsilon_M[\mathbf{x}_{\text{det}}])$ for the angles in across-track direction and along-track (in-flight)-direction, respectively. Because of the polychromatic approach, we are allowed to replace \mathbf{x}_{det} by r_{det} . Now, it is important to realize that these angles are the *centers* of the response function: the detector pixel receives light from a certain angular region $S_0[\mathbf{x}_{\text{det}}]$. The region will resemble a convex, probably asymmetric, area. The intensity of the response at each point inside the area can be visualized as a two-dimensional asymmetric Gaussian $A[\mathbf{x}_{\text{det}}](\phi, \varepsilon)$. The volume of A is supposed to be normalized and the lines of sight introduced above are defined as the barycenters:

$$M_{\text{tot}} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A[\mathbf{x}_{\text{det}}](\phi, \varepsilon) d\phi d\varepsilon = 1; \quad (337)$$

$$\varphi_M[\mathbf{x}_{\text{det}}] = \int_{-\infty}^{\infty} \phi \left[\int_{-\infty}^{\infty} A[\mathbf{x}_{\text{det}}](\phi, \varepsilon) d\varepsilon \right] d\phi; \quad (338)$$

$$\varepsilon_M[\mathbf{x}_{\text{det}}] = \int_{-\infty}^{\infty} \varepsilon \left[\int_{-\infty}^{\infty} A[\mathbf{x}_{\text{det}}](\phi, \varepsilon) d\phi \right] d\varepsilon; \quad (339)$$

$$(340)$$

The boundary of the area is defined as the isoline of zero intensity ∂S_0 ; no light from outside the area will reach this detector pixel. Note that we consider here the completely corrected signal; necessary corrections like straylight have already been performed.

At each instantaneous moment in time t_0 , the detector pixel is receiving light from a certain area on the surface of the Earth, expressed in geocentric (or, ultimately, geodetic) latitude and longitude. The projection from azimuth and elevation angles towards these co-ordinates $(\delta, \vartheta) = T(\phi, \varepsilon)$ is well-defined. We call the projection of the response function A at t_0 the *staring* or *instantaneous* field of view $B[\mathbf{x}_{\text{det}}, t_0](\delta, \vartheta) = T(A[\mathbf{x}_{\text{det}}](\phi, \varepsilon))$. Translated to Cartesian co-ordinates on the surface of the Earth, the extent of B is about [5.8,4.3,4.3,21.7] km across-track and [7.2,4.3,4.3,14.4] km along-track for pixel (512,512) of the four detectors, respectively. An example of such a response function can be seen in figure 61.

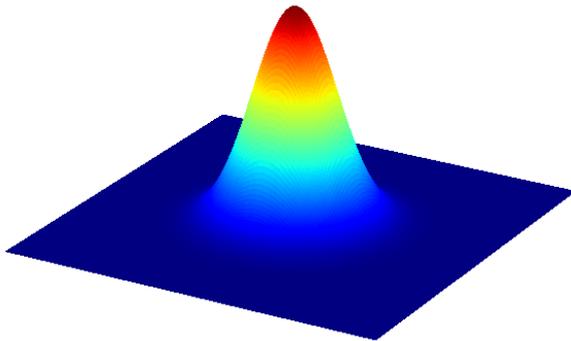


Figure 61: Surface plot of normalized asymmetric 2D-Gaussian; co-ordinates are latitude and longitude.

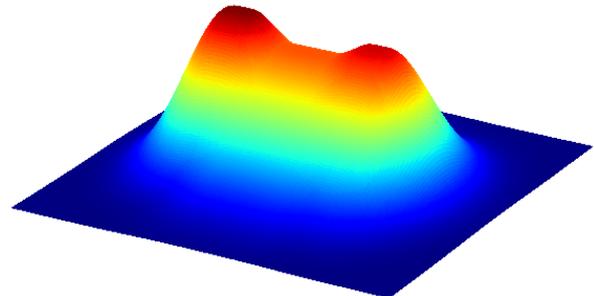


Figure 62: Surface plot of convoluted asymmetric 2D-Gaussians: response of a detector pixel during one exposure.

- Now, we consider the field of view during one exposure from t_0 to t_1 . During this interval, the instrument moves (per definition) along-track. That means that the entire response function is convoluted along a path from $(\delta(t_0), \vartheta(t_0))$ toward $(\delta(t_1), \vartheta(t_1))$ where the latitudes and longitudes are defined inside $T(S_0)$:

$$\phi[\mathbf{x}_{\text{det}}, t]_{t_0 \leq t \leq t_1}(\delta, \vartheta) = \int_{-\infty}^{\infty} B[\mathbf{x}_{\text{det}}, \tau](\delta, \vartheta) \cdot \mathbf{I}(t - \tau) d\tau \quad (341)$$

where $\mathbf{I}(t)$ equals one for t between t_0 and t_1 and is zero elsewhere. If the velocity of the instrument $v(t)$ were constant and the Earth a perfect sphere, then the projection $B(t)$ would be regular and $\phi(t)$ would resemble an perfectly block-convoluted Gaussian, thus elongated in along-track direction with a constant maximum between $T(\phi_M(t_0), \varepsilon_M(t_0))$ and $T(\phi_M(t_1), \varepsilon_M(t_1))$. Since that is not the case, the response function for one exposure time will look similar as in figure 62.

- We assume that the signal has been perfectly corrected for the smear. If that is not the case, then the signal in each row contains some signal from all other rows. If visualized, this would mean that the Gaussian were extremely long-tailed in the across-track direction. Note that for time-varying scenes, the current smear correction algorithm is not perfect.

- Once the image of an exposure period has been transported to the storage region, several detector pixels are binned into one image pixel. That means that the individual response functions are simply added, thus becoming extended in across-track (longitudinal) direction:

$$\phi[\mathbf{x}_{\text{img}}, t]_{t_0 \leq t \leq t_1}(\delta, \vartheta) = \sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}} \dots \infty} \int_0^\infty B[\mathbf{x}_{\text{det}}, \tau](\delta, \vartheta) \cdot \mathbf{I}(t - \tau) d\tau \quad (342)$$

The resulting shape in across-track direction will probably contain some local minima, while the local maxima associated with detector pixels well 'inside' the image pixel will be more or less the same, see figure 63.

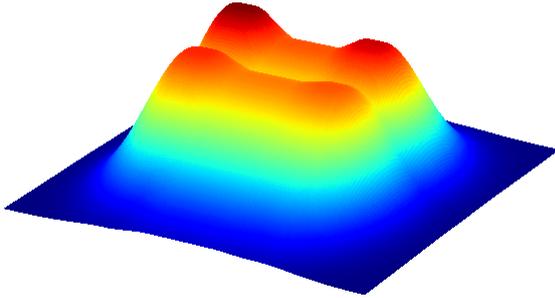


Figure 63: Surface plot of summed and convoluted asymmetric 2D-Gaussians; response of an image pixel during one exposure.

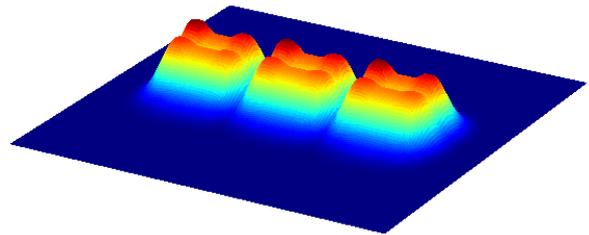


Figure 64: Surface plot of double-summed and convoluted asymmetric 2D-Gaussians; response of a co-added image pixel: effectively, a ground pixel.

- The image pixels are then co-added together with images from other exposures in a co-addition period. This gives for the response function:

$$\phi[\mathbf{x}_{\text{img}}, t]_{t_0(0) \leq t \leq t_1(N_{\text{coadd}})}(\delta, \vartheta) = \sum_{j=1}^{N_{\text{coadd}}} \sum_{\mathbf{x}_{\text{det}} \in \mathbf{x}_{\text{img}} \dots \infty} \int_0^\infty B_j[\mathbf{x}_{\text{det}}, \tau](\delta, \vartheta) \cdot \mathbf{I}_j(t - \tau) d\tau \quad (343)$$

Here B_j and \mathbf{I}_j are the responses and block functions, respectively, for a given exposure time period j . Since we are performing a summation of separate response functions here, the result will probably not be a perfect elongated (in along-track direction) variant of the function visualized in figure 62; instead, the function would resemble the one in figure 63 replicated a few times in the longitudinal dimension (see figure 64):

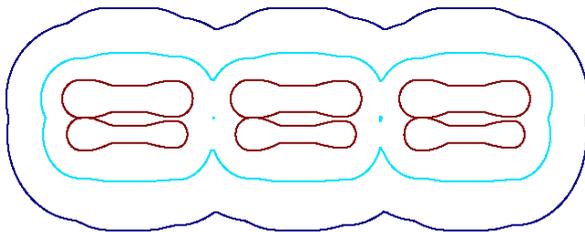


Figure 65: Contour plot of double-summed and convoluted asymmetric 2D-Gaussians, indicating possible ground pixel boundaries.

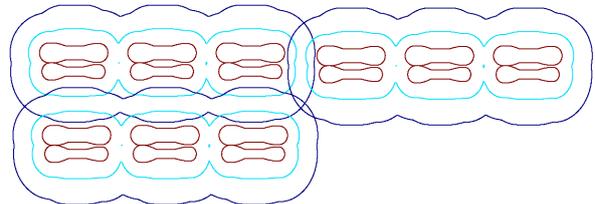


Figure 66: Contour plots of three double-summed and convoluted asymmetric 2D-Gaussians, indicating a tiling in both across-track and along-track direction. The blue contours are useless; the yellow contours leave gaps between ground pixels; the red contours overlap significantly.

We have formally constructed the response function on one image pixel during one co-addition. Now we address the problem how to obtain the ground pixel extent. Besides the constraint that the relation to other ground pixels must be taken into account, there is the choice of the measure criterion of a ground pixel.

- On the one hand, we can draw isolines (these are curves connecting the points of the same height). A choice of isoline will result in a 2D-curve as a function of latitude and longitude on the Earth's surface; see figure 65.
- On the other hand, we can define a certain shape (a rectangle, ellipse, tile) and acquire the radius/perimeter such that the intersection of this particular shape and the response function will contain a certain fraction of the total volume of the response function. As a variant, we can square the height of the response function first; this leads to an 'integrated energy' criterion.

If we follow the first approach, then the isolines of neighboring (i.e. row or co-addition period) will certainly not fill up the Earth's surface plane in an ordered way: either the intersections are not empty (regions of overlap exist), or the union does not equal the whole surface (there are regions that are not covered by any proposed ground pixel). See figure 66. Concerning the second approach: only a few possibilities exist for tiling a plane by regular polygons (non-polygons like ellipses immediately fail the intersection/union-test). Of these polygons, hexagons and rhombuses cannot lie in an orthogonal pattern. This leaves rectangles as the only option. Note that this means that the resulting fraction of rectangle and (squared) response function will be a result, not a constraint holding for each ground pixel.

Of course, the demand that forbids overlap and/or gaps can be dropped and for particular L2-applications this might be useful. However, for general purposes, we provide only the standard rectangular tiling based on LOS-geocentric co-ordinates and timestamps.

27 Geometrical algorithms

The main goal of the geometrical algorithms is to correlate each detector or image row r to the latitude δ and longitude ϑ of the corresponding ground pixel. Or in other words, to determine from which location of the Earth's surface (or more precisely: column of atmosphere) each detector is receiving radiation during a measurement.

In order to perform this calculation, the following parameters are required; working from the detector pixel to the ground:

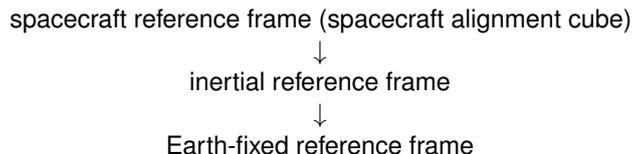
1. Line-of-sight angles (see Section 26.4.8), i.e., the azimuth angle ϕ and elevation angle ε of each detector pixel, which are measured with respect to the optical alignment cube (OAC) during the calibration campaign. The OAC is aligned with the payload reference frame.
2. Rotations from the OAC to the spacecraft alignment cube (SAC), which are measured after the instrument has been integrated with the spacecraft. The SAC is aligned with the spacecraft reference frame.
3. Attitude of the spacecraft reference frame with respect to the inertial reference frame, which is continuously measured in-flight by the star tracker subsystem (STR).
4. Position of the spacecraft in the Earth-fixed reference frame, which is continuously measured in-flight by the global navigation satellite system (GNSS).

The applicable reference frames are explained in Section 26.1. Subsequently, from the location of a ground pixel, the azimuth angle ϕ and zenith angle θ of the spacecraft are determined, as well as the azimuth and zenith angles ϕ_0 and θ_0 , respectively, of the Sun. Other geometrical algorithms are used to calculate the orbit phase and the location of the sub-satellite point (SSP) or to determine if a measurement may be affected by sun glint, a spacecraft maneuver, a solar eclipse or the South Atlantic Anomaly.

27.1 Ground pixel position

The position of a measurement on Earth i.e., the center of a ground pixel, in terms of longitude ϑ and latitude δ , is given by the intersection of the line of sight vector with the reference ellipsoid. This line of sight vector is determined by the direction of the barycenter of the measurement polychromatic spatial response function as described in Section 26.4.8. The line of sight vector will need to be sequentially transformed between the following reference frames:

payload reference frame (optical alignment cube)
↓



For the transformation steps within the vicinity of the spacecraft, only rotations are taken in to account while translations are ignored. This can be safely applied as the translations within the spacecraft only amount to meters while the resolution on-ground is in the order of kilometers. To be able to transform the line of sight from the payload reference frame to the spacecraft reference frame, this LOS direction vector \mathbf{I}_{PRF} first needs to be converted to a unit direction vector $\hat{\mathbf{I}}_{\text{PRF}}$. Using the definition of the detector pixel LOS azimuth and elevation from Section 26.1.11 the LOS unit vector ($r = \sqrt{x^2 + y^2 + z^2} = 1$) is determined as

$$\hat{\mathbf{I}}_{\text{PRF}} = \begin{bmatrix} \hat{l}_{\text{PRF},x} \\ \hat{l}_{\text{PRF},y} \\ \hat{l}_{\text{PRF},z} \end{bmatrix} = \begin{bmatrix} + \sin \varepsilon \\ - \cos \varepsilon \sin \phi \\ + \cos \varepsilon \cos \phi \end{bmatrix}. \quad (344)$$

The LOS unit vector can then be transformed from the payload reference frame to the spacecraft reference frame as described in Section 26.2.1. To determine the intersection of a LOS in the spacecraft reference frame with the WGS84 Earth reference ellipsoid, the LOS first has to be transformed to the inertial reference frame with the rotation matrix from Section 26.2.3 to yield the direction of this unit LOS vector in the inertial reference frame. Subsequently it has to be transformed to the Earth-fixed reference frame as described in Section 26.2.5.

The position vector of the spacecraft in the Earth-fixed reference frame (which is measured by the GNSS system) together with this unit LOS direction vector in the Earth-fixed reference frame determines the line of sight in the Earth-fixed reference frame. The intersection of this resulting line of sight is then taken with the WGS84 Earth reference ellipsoid, as described in Section 26.3. Since this yields two intersection points, care has to be taken to determine which of the two intersection points is the one which is needed. This intersection point is then converted from geocentric Cartesian to geodetic coordinates as described in Section 26.2.6, to yield the final ground pixel location in latitude δ and longitude ϑ .

27.1.1 Ground pixel corner points

The extent of a ground pixel is ill-determined due to the fact that an arbitrary choice has to be made about which extent of the measurement polychromatic spatial response function is representative for the TROPOMI instrument. Suggestions of possible definitions are given in Section 26.4.9 (together with the relation to the issue of inter-band and intra-band co-registration) and more extensively in Section 26.4.10. During on-ground calibration the instantaneous line of sight (ILOS) is determined for each detector pixel under static conditions. The instantaneous line of sight is the barycenter of the pixel polychromatic spatial response function (see Sec. 26.4.8). In flight, the line of sight of one detector pixel sweeps over a range of ground positions during one exposure (blue peaks in the middle of Figure 67). The exposures of one co-addition period are added up to one *measurement*, depicted as a dark blue envelope in the figure. The center time T_{center} of the measurement in combination with the ILOS of the detector pixel, is used to determine the center point of a ground pixel with the geolocation algorithms.

For the center points, the lines of sight are averaged in the spectral direction per detector band. This transforms the wavelength dependence of the geolocation into a detector band dependence. Polarization effects are not measured and thus not accounted for. In the following step, the lines of sight are binned in the spatial direction, according to the binning scheme in Table 12. That is, the lines of sight of a group of binned pixels are averaged. The resulting averaged LOS parameters (azimuth, elevation) are then used to determine the ground pixel center point. This ground pixel is now correlated to an image pixel, consisting of a number of binned detector pixels.

To determine the area that a ground pixel extends, its corner points have to be determined. This is done by taking the groups of binned LOS values in the spatial direction on the detector, and interpolating neighboring detector (i.e. unbinned) pixel LOS values to obtain the LOS edges of these groups. The azimuth and elevation curves versus detector pixel are expected to be sufficiently smooth to be able to safely apply this method. The interpolated values for azimuth and elevation are then used to determine the corner point lines in along-track direction (dotted horizontal lines in the right panel of Figure 67). These lines fix the corner points distribution in across-track direction.

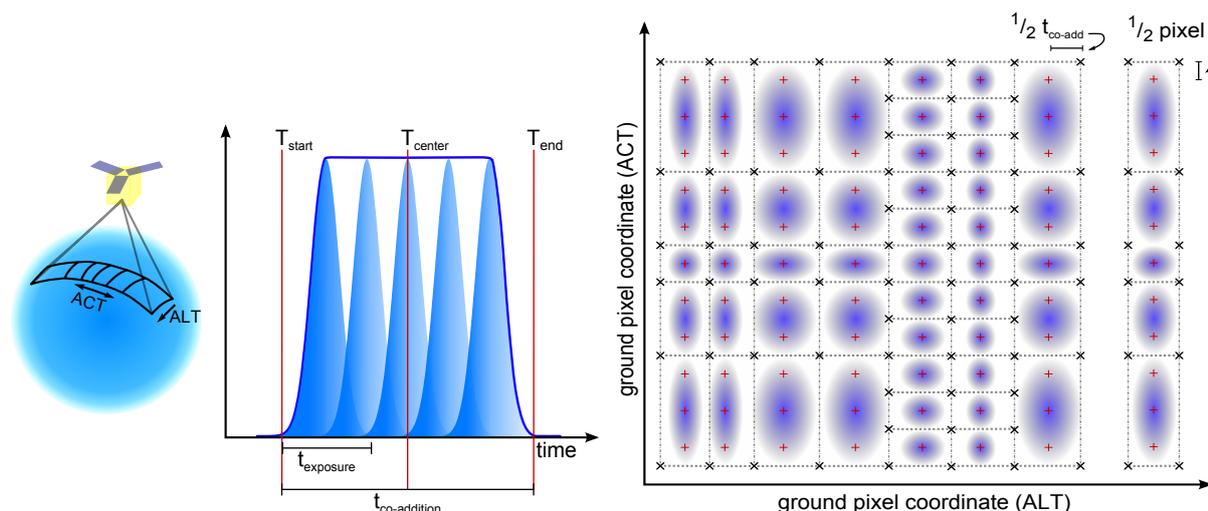


Figure 67: The along-track (ALT) and across-track (ACT) directions along one scanline (left). The movement of the instantaneous line of sight of one detector pixel during one exposure (blue peaks) added to one measurement during the co-addition period (dark blue envelope). The center point for the measurement is determined from T_{center} (middle). The inter- and extrapolation of the center times and the lines of sight resulting in the corner points definition (right), for a single measurement and for a sequence.

To determine the distribution of the corner points in along-track direction, the corner point lines in across-track direction (dashed-dotted vertical line in the illustration) are obtained by interpolation between the previously determined center points. The interpolation in along-track direction is achieved by taking the average of the timestamps of two following measurements in a sequence, and then interpolating the position and attitude coordinates of the spacecraft. By using these interpolated input parameters along with the interpolation over the lines of sight of the binned image pixels, one can determine the corner points of each ground pixel as visualized in the right schematic of Figure 67.

To determine the most East and West corner points of the scanline, the LOS of the last detector pixel is extrapolated in across track direction to yield the bounding lines of sight. To determine the start corner points of the first scanline, and the end corner points of the last scanline in a measurements sequence, the measurement time is extrapolated. The same procedure is used when a measurement in the series is missing, faulty or corrupted, which effectively divides a measurement sequence in multiple sequences. If there is only a single measurement, the start and end time of the measurement are used to determine the timestamps of the bounding corner points.

These extrapolated timestamps are then used in combination with the inter-/extrapolated lines of sight in across-track direction to obtain the start and end corner point boundaries.

Concluding, the method to compute ground pixel corner points has the following properties:

- Since these corner points are determined directly from interpolated values for the lines of sight, time, position and attitude parameters, only one grid of corner points has to be determined, once. As a result, the ground pixel tiles in this grid will neither have overlap, nor gaps between them.
- The keystone effect is accounted for by using this method, since the corner points of the ground pixels are defined by direct intersection of the interpolated lines of sight with the Earth reference ellipsoid.
- Due to the divided approach for the center- and corner points determination, the center points do not exactly lie at the spatial interpolation points of the corner points, nor are the corner points located at the spatial inter-/extrapolation of the center points.
- The spatial response functions of the pixels are not needed for the calculation of the ground pixel corner point positions: only the LOS angles of the rows are.

27.2 Satellite position

Using the position of the satellite, the sub-satellite point (SSP) and the relative position of the spacecraft in the orbit, quantified by the orbit phase, are determined as described below.

27.2.1 Satellite position and velocity interpolation

The position and velocity of the satellite at any moment in time is determined by interpolating ephemeris data, which include the position and velocity Cartesian components (x,y,z) at certain GPS measurement or on-board time (OBT) instances. Since the orbit can be approximated by an ellipse, one could fit an ellipse through some of these ephemeris position points around the requested time, and so interpolate the position for the requested time geometrically. However, in reality the orbit is not an ellipse but on top of this approximation there are secular, long-period and short-period perturbations. By using just a fitted ellipse for the interpolation the velocity would always point outward of the ellipse while the interpolation position would always lay outward of the used ephemerides.

However, in reality the velocity could also act inwards of the ellipse and the resulting position could lay inward of the ellipse. Therefore, a cubic Hermite spline interpolation method is used that fits a third-degree polynomial through the ephemeris points before (subscript 0) and after (subscript 1) the requested time, and uses the velocity and position of these points. The interpolation is done separately for each position p and velocity v Cartesian component. First, four polynomial coefficients (subscripts 0-3) are determined as

$$c_0 = p_0 , \quad (345)$$

$$c_1 = \Delta t v_0 , \quad (346)$$

$$c_2 = 3(p_1 - p_0) - \Delta t(2v_0 + v_1) , \quad (347)$$

$$c_3 = 2(p_0 - p_1) + \Delta t(v_0 + v_1) , \quad (348)$$

where $\Delta t = t_1 - t_0$ is the difference in time between the two ephemeris points. To interpolate to the requested time t , this time is converted to a relative fraction of the interval as

$$t_{\text{rel}} = \frac{t - t_0}{\Delta t} , \quad (349)$$

and the position and velocity component can then be obtained by using

$$p = c_0 + c_1 t_{\text{rel}} + c_2 t_{\text{rel}}^2 + c_3 t_{\text{rel}}^3 , \quad (350)$$

$$v = \frac{c_1 + 2c_2 t_{\text{rel}} + 3c_3 t_{\text{rel}}^2}{\Delta t} . \quad (351)$$

27.2.2 Satellite attitude interpolation

To determine the attitude of the spacecraft at any given time, the attitude measurements as unit quaternion rotation from the inertial to the spacecraft reference frame are interpolated linearly, for all four components separately, as

$$q = \frac{(t_1 - t)q_0 + (t - t_0)q_1}{t_1 - t_0} , \quad (352)$$

after which it is normalised, for a valid reversible rotation.

27.2.3 Sub-satellite point and altitude

The SSP is defined as the intersection of the line from the position of the spacecraft normal to the surface of the WGS84 Earth reference ellipsoid, see Figure 53). It is described by the longitude and geodetic latitude of the spacecraft in the Earth-fixed reference frame. The altitude of the spacecraft is defined as the distance between the spacecraft and the sub-satellite point.

To obtain the above SSP parameters, one first has to know the position of the spacecraft in the Earth-fixed reference frame (measured by the GNSS), after which the intersection point with the WGS84 Earth reference ellipsoid can be determined. The conversion from the Earth-fixed reference frame geocentric Cartesian coordinates to geodetic coordinates is then performed as described in Section 26.2.6.

27.2.4 Orbit phase

The orbit phase is defined as $1/(2\pi)$ times the angle in radians traversed by the spacecraft since spacecraft midnight as seen from the center of the Earth. Spacecraft midnight is the point on the night side of the Earth where the spacecraft crosses the orbital plane of the Earth about the Sun. This makes the orbit phase a quantity that runs from 0 to 1, while the spacecraft moves between each spacecraft midnight. Note that the orbit phase depends almost linearly on elapsed time, but not exactly, since the Sentinel-5p orbit is not a perfect circle. See Figure 68 for a graphical illustration of the orbit phase definition.

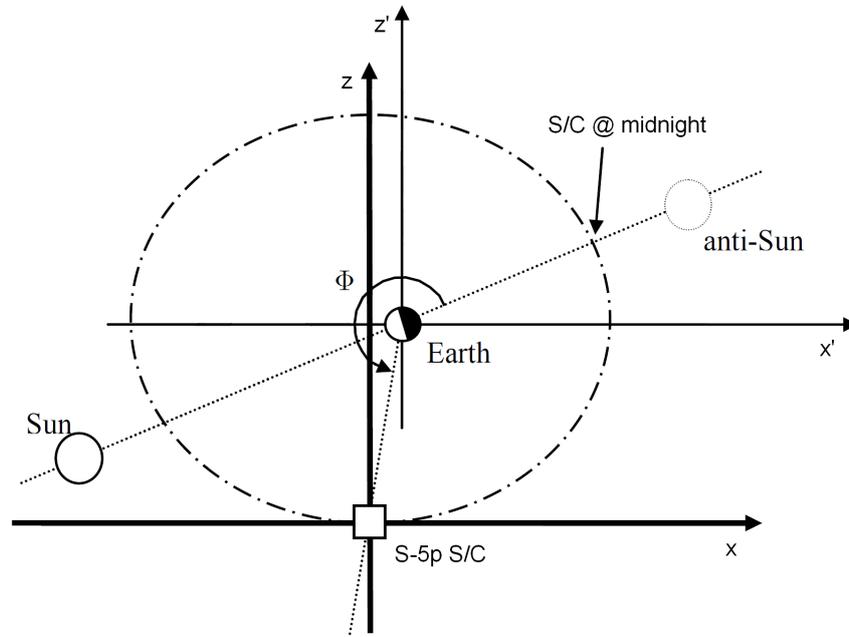


Figure 68: Definition of the orbit phase Φ .

To determine the orbit phase Φ at a measurement time instance, first the position of the Sun is determined in the true-of-date reference frame as described in Section 27.3.1, which is converted to the inertial reference frame by multiplying with rotation matrix $[\mathbf{Q}(t)]^T$ to subtract the precession and nutation since the epoch J2000.0, see section 26.2.5. The positions of the Earth (i.e., the origin) and the Sun are then transformed to the orbital reference frame as derived in Section 26.2.8. These position vectors are then both projected onto the orbital plane by setting the first coordinate (T) in the local orbital reference frame, which is the coordinate perpendicular to the orbital plane, to 0. The resulting vectors are then translated such that the center of the Earth is at the origin instead of the center of the spacecraft. The orbit phase Φ is now determined as

$$\Phi = \frac{\arctan2(z_{S/C,Orb}, y_{S/C,Orb}) - \arctan2(-z_{Sun,Orb}, -y_{Sun,Orb})}{2\pi}, \quad (353)$$

in which the $\arctan2$ function determines an angle in the range $(-\pi, \pi]$ instead of the normal \arctan function which has results within $(-\pi/2, \pi/2]$. Finally, the integer 1 needs to be subtracted or added until Φ lies in the range $[0, 1)$.

27.3 Solar angles

For the solar angles algorithms, first the location of the Sun is determined. Following, the Sun's LOS angles in the payload reference frame, the velocity scalar of the spacecraft towards the Sun, and the LOS from the ground pixel towards the Sun and the spacecraft can be determined, which are described below.

27.3.1 Position of the Sun in the true-of-date reference frame

The Sun's position (x, y, z) can be determined in the true-of-date reference frame using [RD18]. The reference describes low-precision (1 arcminute) formulae for planetary positions, including the Sun, and includes a large number of coefficients to be used with these formulae. The algorithms described use as input only the Julian

date (in UT or Greenwich Mean Time (GMT)) since J2000, assigned t , from which the time T in Julian centuries since the epoch 1900 is determined as

$$T = \frac{t}{36525} + 1 . \quad (354)$$

To determine the position of the Sun, the following fundamental arguments of the Moon (Mo), the Sun (S), Venus (V), Mars (Ma) and Jupiter (J) are needed:

$$L_{\text{Mo}} = 0.606434 + 0.03660110129t , \quad (355a)$$

$$\Omega_{\text{Mo}} = 0.347343 - 0.00014709391t , \quad (355b)$$

$$L_{\text{S}} = 0.779072 + 0.00273790931t , \quad (355c)$$

$$G_{\text{S}} = 0.993126 + 0.00273777850t , \quad (355d)$$

$$G_{\text{V}} = 0.140023 + 0.00445036173t , \quad (355e)$$

$$G_{\text{Ma}} = 0.053856 + 0.00145561327t , \quad (355f)$$

$$G_{\text{J}} = 0.056531 + 0.00023080893t , \quad (355g)$$

where L is the mean longitude and G is the mean anomaly of a certain planet, while Ω is the longitude of the lunar ascending node. Then, the geocentric equatorial coordinates right ascension (α), declination (δ) and geocentric distance (ρ) are determined as

$$\alpha = L + \arcsin \left[\frac{W}{\sqrt{U - V^2}} \right] , \quad (356a)$$

$$\delta = \arcsin \left(\frac{V}{\sqrt{U}} \right) , \quad (356b)$$

$$\rho = \bar{\Delta} \sqrt{U} , \quad (356c)$$

where $\bar{\Delta}$ is a scaling factor which is 1.00021 for the Sun, and U, V, W are intermediaries which can be determined using (co)sine series with coefficients listed in the Appendix of [RD18] in combination with T and the fundamental arguments L, G , and Ω of above. The coordinates (α, δ, ρ) are simply the longitude, geocentric latitude and radius (ϑ, δ', r) in the true-of-date reference frame which can be converted to Cartesian components ($x_{\text{Sun, TODRF}}, y_{\text{Sun, TODRF}}, z_{\text{Sun, TODRF}}$) as explained in Section 26.2.6. The Earth-Sun distance $D_{\text{Earth-Sun}}$ is then evaluated as

$$D_{\text{Earth-Sun}} = \sqrt{x_{\text{Sun, TODRF}}^2 + y_{\text{Sun, TODRF}}^2 + z_{\text{Sun, TODRF}}^2} , \quad (357)$$

which can then be divided by $AU = 149,597,870,700$ m to convert from meters to Astronomical Units. One AU is the mean orbital distance from the Earth to the Sun.

27.3.2 Solar line of sight in the Sun port reference frame

Using the ephemeris of the Sun, the position of the spacecraft in the inertial reference frame, and the attitude of the spacecraft reference frame with respect to the inertial reference frame, one can determine the azimuth ϕ and elevation ε of the line of sight from the spacecraft to the Sun in the Sun port reference frame. The angles ϕ and ε are defined here in the same way as described for the payload reference frame, Section 26.1.11, but now with respect to the Sun port reference frame. To this end the position of the spacecraft in the Earth-fixed reference frame, as measured by the GNSS, is transformed to the inertial reference frame, as described in Section 26.2.5.

The Sun's position can be determined in the true-of-date reference frame as described in Section 27.3.1. This position vector can then be transformed to the inertial reference frame by deducting the precession and nutation since J2000.0 as described in Section 26.2.5, which means multiplying by the transpose of the rotation matrix $\mathbf{Q}(t)$. Then, the position vector is transformed to the spacecraft reference frame as described in Section 26.2.3. Then, it is transformed to the payload reference frame as described in Section 26.2.1, by multiplying with the transpose of the rotation matrix $\mathbf{R}_{\text{zyx, PRF} \rightarrow \text{SRF}}$. Finally, it is transformed to the Sun port reference frame, as described in Section 26.2.9. The solar elevation ε and azimuth ϕ in the Sun port reference frame can then be determined as

$$\phi_{\text{Sun, SPRF}} = \arctan 2(-y_{\text{Sun, SPRF}}, z_{\text{Sun, SPRF}}) , \quad (358a)$$

$$\varepsilon_{\text{Sun, SPRF}} = \arcsin(x_{\text{Sun, SPRF}}) , \quad (358b)$$

in which $\arctan 2$ ensures that the solar azimuth angle is evaluated as $-\pi < \phi_{\text{Sun, SPRF}} \leq \pi$.

27.3.3 Velocity of spacecraft towards Sun

The position and velocity components of the spacecraft follow from the GNSS measurements, and are defined in the Earth-fixed reference frame. These are transformed to the inertial reference frame as described in Section 26.2.5. Using the Sun's position in the inertial reference frame as determined in the previous section, the position vector $\mathbf{p}_{S/C \rightarrow \text{Sun,IRF}}$ of the Sun relative to the spacecraft in the inertial reference frame is now determined as

$$\mathbf{p}_{S/C \rightarrow \text{Sun,IRF}} = \mathbf{p}_{\text{Sun,IRF}} - \mathbf{p}_{S/C, \text{IRF}} , \quad (359)$$

with which the amplitude of the velocity $\mathbf{v}_{S/C \rightarrow \text{Sun,IRF}}$ of the spacecraft in the direction of the Sun is computed as

$$\|\mathbf{v}_{S/C \rightarrow \text{Sun,IRF}}\| = \frac{(\mathbf{p}_{S/C \rightarrow \text{Sun,IRF}}, \mathbf{v}_{S/C, \text{IRF}})}{\|\mathbf{p}_{S/C \rightarrow \text{Sun,IRF}}\|} , \quad (360)$$

in which the length of the position vector of the Sun relative to the spacecraft in the inertial reference frame is defined as

$$\|\mathbf{p}_{S/C \rightarrow \text{Sun,IRF}}\| = \sqrt{x_{S/C \rightarrow \text{Sun,IRF}}^2 + y_{S/C \rightarrow \text{Sun,IRF}}^2 + z_{S/C \rightarrow \text{Sun,IRF}}^2} . \quad (361)$$

27.3.4 Spacecraft and Sun lines of sight from ground pixel

Level-2 data processors need information on the lines of sight from the ground pixel position to the spacecraft and to the Sun, in the topocentric reference frame. These are defined by the solar azimuth ϕ_0 and zenith θ_0 angles for the incident sunlight, and spacecraft azimuth ϕ and zenith θ angles for the scattered sunlight, and are indicated in Figure 69. With these angles the level-2 data processors can for instance determine the scattering angle Θ .

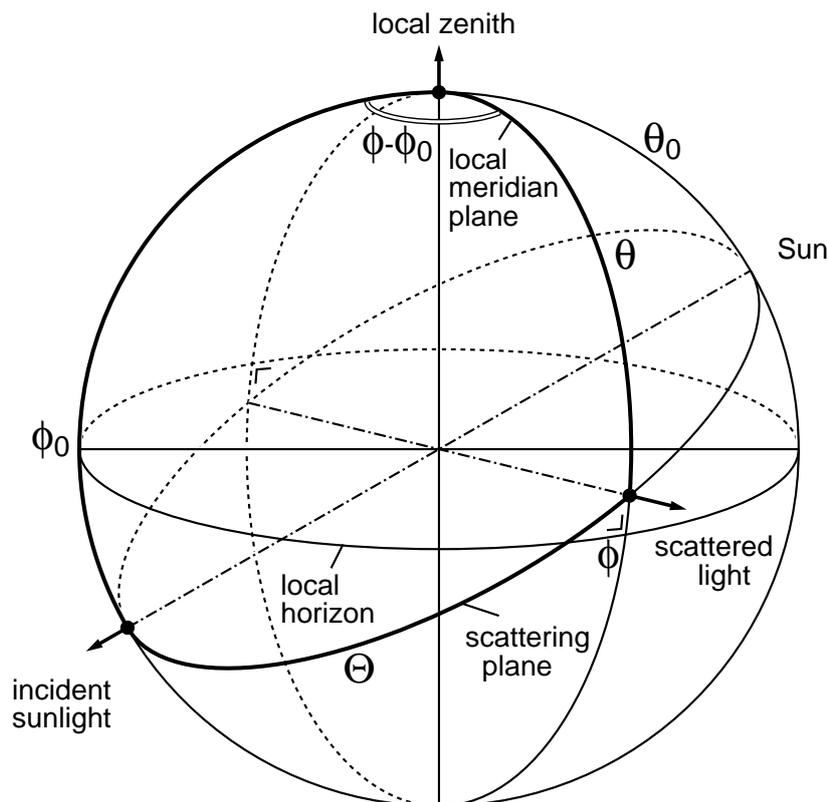


Figure 69: Definition of the LOS zenith θ and azimuth ϕ angles from the ground pixel location to the spacecraft and Sun (θ_0, ϕ_0), and scattering angle Θ .

In order to determine these LOS angles for the spacecraft, the position of the spacecraft in the Earth-fixed reference frame as measured by the GNSS subsystem is transformed to the topocentric reference frame, as described in Section 26.2.7.

To determine the LOS angles for the Sun, the position of the Sun in true-of-date reference frame is computed as indicated in Section 27.3.1. Then, this position is transformed to the Earth-fixed reference frame by first multiplying with $[\mathbf{Q}(t)]^T$ to get to the inertial reference frame and then with $\mathbf{W}(t)\mathbf{R}(t)\mathbf{Q}(t)$ (since this total matrix was already calculated) as described in Section 26.2.5. Then the position is further transformed to the topocentric reference frame as explained in Section 26.2.7.

The LOS angles are then determined as

$$\theta_0 = \arctan \frac{\sqrt{x^2 + y^2}}{z}, \quad (362a)$$

$$\phi_0 = \arctan 2(-x, -y), \quad (362b)$$

$$\theta = \arctan \frac{\sqrt{x^2 + y^2}}{z}, \quad (362c)$$

$$\phi = \arctan 2(x, y), \quad (362d)$$

in which the $\arctan 2$ determines an angle in the range $-\pi - \pi$ instead of the normal \arctan function which results in an angle from $-\pi/2 - \pi/2$. The minus signs in front of x and y for the solar azimuth thus ensure that the azimuth angle of the incident ray of the Sun is determined, like indicated in Figure 69, and not of the Sun itself.

27.3.5 Atmospheric Refraction of Light

All geolocation analysis so far has been done assuming there is no refraction of the light beam due to the Earth's atmosphere. However, in reality, this does occur, which changes the solar and viewing angles as well as the position of the ground pixels. Since each point in the variable atmosphere has its own density, pressure, temperature and humidity (which are influenced by current local weather conditions) it also has its own refraction coefficient. Thus, to precisely account for all atmospheric refraction effects, an atmospheric model would have to be set up, through which the 3D light beam path, with a certain wavelength, would have to be integrated. Unfortunately, this would be too computationally intensive to implement in detail, as it would cost far too much CPU-time.

However, the effect of atmospheric refraction at zenith angles of 90 degrees can reach approximately half a degree, and thus should be corrected for. To include this effect, some assumptions thus have to be made. Using a simple model for the atmosphere that is concentrically homogeneous, the same conditions apply at the same altitude anywhere on Earth. Furthermore, assuming an observation point at sea-level with an atmospheric pressure of 1010 millibars and a temperature of 10° Celsius, where the refraction is calculated for a yellow light beam in the visible part of the electromagnetic spectrum. Then, an empirical equation that approximates the refraction R in arcminutes can be set up [RD19] based on the true altitude h in degrees:

$$R = \frac{1.02}{\tan \left(h + \frac{10.3}{h+5.11} \right)}, \quad (363)$$

in which the true altitude h is connected to the true zenith angle θ as

$$h = \pi - \theta. \quad (364)$$

The apparent zenith angle at which the light beam reaches the ground pixel location is now determined from

$$\theta_a = \theta - R. \quad (365)$$

as the light beam is always refracted towards the zenith. That is, the zenith angle decreases during its path through the atmosphere from top to bottom.

This empirical formula is accurate to about 0.15 arcminutes for true altitude angles h smaller than 3 degrees, while for angles more than 5 degrees it is accurate to the arcsecond level. Resulting from the assumptions, the azimuth angle has no refraction. Plenty of these approximating equations exist (Bennet, Meeus, Explanatory Supplement to the Astronomical Almanac), but were all verified to give similar results.

The atmospheric refraction correction can be turned on or of in the configuration.

28 Wavelength characterization

Each detector pixel is associated with a particular wavelength. Basically, this wavelength is a monotonously increasing function of the detector column number. However, the relationship between detector pixel and wavelength depends also on:

- detector row number, due to the ‘spectral smile’;
- spacecraft velocity, due to the Doppler effect;
- OBM temperature or temperature gradient (however note that the temperature within the TROPOMI instrument is stabilized);
- inhomogeneous slit illumination, due to subpixel scenery variations.

The spectral smile cannot be neglected and has to be taken into account in the wavelength characterization, which means that each detector row is assigned a different wavelength scale. Doppler shift is only important for cases where the speed of the detector towards or away from the light source is non-negligible; that is, only for irradiance measurements. The other effects are expected to be small (temperature), or (inhomogeneous slit illumination) affect the measured radiance in such a manner that cannot be dealt with in the L01b processor because a complete model of the atmosphere is needed and is not available. Therefore, a wavelength calibration is only performed for irradiance measurements, as described in the following.

28.1 Initial wavelength assignment

As explained above, the wavelength characterization for radiance measurements can be considered to be independent of measurement. Therefore, the Level-1b radiance product will contain a single ‘image’ containing the wavelength as a function of row and column number: this is sufficient for display purposes and can serve as a starting point for the wavelength calibration performed in the Level-1b to Level-2 processors. It also serves as a starting point for the wavelength calibration for the irradiance in the L01b, which includes the Doppler shift correction (Section 28.2) and the wavelength calibration (Section 28.3).

The initial wavelength scale is determined by the position and orientation of the optics, the slit, the gratings, and the detectors themselves, and is established during on-ground calibration in the form of Chebyshev expansion coefficients $a_n[r_{\text{det}}]$. In the initial annotation algorithm, each pixel is assigned a wavelength $\lambda_{[\mathbf{x}_{\text{det}}]}$ based on this polynomial expansion:

$$\lambda_{[\mathbf{x}_{\text{det}}]} = \sum_{n=0}^N a_n[r_{\text{det}}] \cdot T_n \left(2 \frac{c_{\text{det}} - c_{\text{min}}}{c_{\text{max}} - c_{\text{min}}} - 1 \right), \quad (366)$$

in which $T_n(x)$ is the n th Chebyshev polynomial (see Appendix A), N is the order of the approximation, and c_{min} and c_{max} are chosen such that $-1 \leq 2(c_{\text{det}} - c_{\text{min}})/(c_{\text{max}} - c_{\text{min}}) - 1 \leq 1$ for each c_{det} . Note that for binned measurements, a binning step must be applied.

28.2 Doppler shift correction

When Sun irradiance measurements are performed, the measured spectrum is affected by non-relativistic Doppler shift (Section 16.1). In order to correct for this the wavelength assignment polynomial coefficients are corrected as follows:

$$a_{n,\text{irr}} = a_n \left(1 - \frac{v}{c} \right), \quad (367)$$

where v is the component of the spacecraft velocity along the direction from the spacecraft to the Sun (taken to be positive when the spacecraft moves away from the Sun), and c is the speed of light in vacuum.

28.3 Irradiance wavelength calibration

The wavelength characterization of the irradiance measurements is carried out by comparing the measured spectra with a reference high-resolution solar spectrum [RD20]. The algorithm is based on the work by [RD21] and [RD22], and is applied to each instrument separately.

Let $E_{\text{ref}}(\lambda)$ be the high-resolution solar irradiance spectrum convolved with the instrument's spectral response function. Although this function is discrete, we consider it here to be continuous by means of a linear interpolation of the discrete values. Consider now the following wavelength scale for the irradiance

$$\lambda_{\text{trial}}[\mathbf{x}_{\text{det}}] = \sum_{n=0}^N a_{n,\text{irr}}[r_{\text{det}}] \cdot (1 + \delta_n[r_{\text{det}}]) \cdot T_n \left(2 \frac{c_{\text{det}} - c_{\text{min}}}{c_{\text{max}} - c_{\text{min}}} - 1 \right), \quad (368)$$

where the $\delta_n[r_{\text{det}}]$ are values to be determined. The best wavelength scale for the irradiance measurement $E_0[\mathbf{x}_{\text{det}}]$ is found by minimizing the following quality function

$$Q(\delta_n[r_{\text{det}}]) \equiv \sum_{c_{\text{det}}} \frac{\{E_0(\lambda[\mathbf{x}_{\text{det}}]) - E_{\text{ref}}(\lambda_{\text{trial}}[\mathbf{x}_{\text{det}}])\}^2}{\sigma^2[\mathbf{x}_{\text{det}}]}. \quad (369)$$

Note: the convolution that yields $E_{\text{ref}}(\lambda)$ needs not be performed each time. It can be performed outside of the L01b processor, and $E_{\text{ref}}(\lambda)$ can be part of the CKD data. An update is needed only when the instrument response function changes. The algorithm to be used in the convolution is described in Appendix B.

29 Quality assessment

In case of errors in one of the algorithms, the pertinent image pixels are marked (“flagged”) as such, invalidating them for use in L01b Processor algorithms, as explained in Section 20.1. In addition, a number of dedicated algorithms are designed to detect other issues that relate to the quality of the measurements. These algorithms do not affect the measured signal or its error, but augment these with the results of these quality assessments, often in the form of additional flags.

Flagging denotes the annotation of individual Level-1b data values with detailed processing information. Generally, these are answers to simple yes/no questions such as “has a processing error occurred for this particular spectral sample?” or “was this measurement performed while the spacecraft was in the path of a solar eclipse?”

Users of the Level-1b data are advised to use these data fields to assess the quality of the Level-1b data and filter it before use. In flag fields, the individual bits of the elements matter. For instance, a particular bit of a flag field may indicate “missing data”, so that a value of 1 (when the flag is said to be “raised” or “set”) signifies “yes”, and a value of 0 (“lowered” or “unset”) signifies “no”. This is in contrast to other data fields, where all the bits combined form a real or countable value. Using bitwise operators and a well-chosen bit mask, a user can tailor the selection criteria for his or her purpose.

In addition to the flags, each image pixel has a “quality number” with values between 0 (lowest quality) and 1 (highest quality). When appropriate, the “quality number” of an image pixel is adapted in any L01b algorithm by multiplying with a “quality factor” (also between 0 and 1). This enables algorithms to give a more refined quality assessment than just “good” or “bad”. Also, in this way pixels with low quality that nevertheless pass all individual flagging thresholds can still be recognized as unfit for scientific use.

29.1 Missing data

In the case of data downlink interruptions, image pixels may have no valid signal value at all. These image pixels are flagged as ‘missing’, and are not used in the L01b Processor algorithms.

29.2 Processing errors

A processing error may occur in one of the algorithms, invalidating the image pixels concerned for further use in calculations. However, these image pixels are still processed in subsequent correction algorithms in the L01b Processor, as explained in Section 20.1.

29.3 Detector pixel quality

The detector pixels quality algorithm labels individual defective image pixels. Defective pixels arise mainly from cosmic radiation and their number will increase during nominal operation. Very few pixels are expected to be defective due to imperfect production. A pixel is flagged if one or more of the following points apply:

- The dark current is out of range.
- The dark current noise is out of range.
- The quantum efficiency is too low.
- The response to increasing light flux is not linear (and not increasing) enough.

A defective pixel is not used for the calculation of correction parameters. For example for the PRNU correction the defective pixels are excluded while ensuring that a sufficient number of pixels remain for the PRNU algorithm to function properly. However, all subsequent L01b Processor algorithms are applied to all image pixels, including the defective ones. The resulting data is not useful for scientific purposes but may still be useful for calibration and monitoring products.

The quality of individual pixels in the above sense is monitored throughout the TROPOMI mission. As this involves multiple orbits, maps of detector pixel quality are derived on a regular basis during in-flight calibration outside the processor and are provided as calibration key data to the L01b Processor. These CKD maps contain the quality factor per detector pixel as numbers between 0 (lowest quality) and 1 (highest quality). From these unbinned (detector) pixel maps, binned (image) pixel maps are constructed. The conversion rule is that the quality factor of a binned pixel is the minimum of the quality factors of the unbinned pixels. If, after binning, the quality factor is below a certain threshold, the L01b Processor will set a flag in the corresponding L01b product map.

29.4 RTS pixels

Random telegraph signal (RTS) refers to the phenomenon where the dark current of pixels is jumping between distinct levels with time. The frequency of these jumps is higher for higher temperature. RTS is mainly caused by cosmic radiation.

In case an image pixel displays RTS behavior, it is not used for the calculation of correction parameters. However, as with defective pixels, all subsequent L01b Processor algorithms are applied to all image pixels, including the ones showing random telegraph signal. The resulting data is not useful for scientific purposes but may still be useful for calibration and monitoring products.

The dark current levels of individual pixels are monitored throughout the TROPOMI mission. As this involves multiple orbits, maps of RTS behavior are derived on a regular basis during in-flight calibration outside the processor and are provided as calibration key data to the L01b Processor. The frequency and size of dark current jumps is translated into a quality factor per pixel, with values between 0 (lowest quality) and 1 (highest quality). An unbinned pixel map of quality factors is the calibration key data input for the L01b Processor. From unbinned (detector) pixel maps, binned (image) pixel maps are constructed. The conversion rule is that the quality factor of a binned pixel is the minimum of the quality factors of the unbinned pixels. If, after binning, the quality factor is below a certain threshold, the L01b Processor will set a flag in the corresponding L01b product map.

29.5 Transient signals

The purpose of the transient pixel flagging algorithm is to identify pixels in a time series of measurements that have singular anomalously high signals. These observed signal spikes are caused by the excess charge being dumped on a detector pixel by particles impinging on the detector surface. The particles – mainly electrons and protons – find their origin in the radiation environment encountered in space. We define transient signals as having the following three properties:

1. The duration of a transient signal is so short that it covers only one single measurement. More specific, it is not expected that the duration is longer than the smallest exposure time.
2. The spatial extent of a transient signal is so small that it only covers one detector pixel.
3. Since a transient signal dumps charge on a pixel, a transient signal only increases and never decreases the amount of signal.

The following section describes a transient pixel flagging algorithm that has been developed to detect signals that have these properties. This algorithm takes place in the processing flow after the binning correction, but before residual correction.

29.5.1 Algorithm description

The algorithm starts with applying a peak filter to the time signal of each individual image pixel ($r_{\text{img}}, c_{\text{img}}$). That is, for each image pixel of a measurement f , a spikeness K is calculated based on that pixel's signal in the preceding and following measurements:

$$K[r_{\text{img}}, c_{\text{img}}, f] = \frac{S_i[r_{\text{img}}, c_{\text{img}}, f]}{S_i[r_{\text{img}}, c_{\text{img}}, f-1]^\alpha \cdot S_i[r_{\text{img}}, c_{\text{img}}, f+1]^{1-\alpha}}, \quad (370)$$

with $\alpha = 0$ for the very first measurement of the granule, 1 for the very last measurement, and 0.5 for all other measurements. With $\alpha = 0.5$, K is the square root of the product of the following two factors: 'current/previous' and 'current/next'. The first factor is large when the pixel has undergone a sudden increase in signal, while the second factor is large when the pixel has undergone a sudden decrease. The expression is largest when both factors are high, meaning that the pixel has undergone a signal increase for the duration of a single measurement. This corresponds exactly with the first property of transient signals. Also the third property is covered by this expression, because a sudden drop in signal will result in $K < 1$.

However, this equation does not test for the second property. For instance, changes in the scenery, covering a group of neighboring image pixels, would also cause the transient pixel flagging algorithm to trigger if it were based on Equation (370) alone. Therefore, after having applied the peak detector to the measured data, the result $K[r_{\text{img}}, c_{\text{img}}, f]$ should be compared with the K of the neighboring pixels. This is done by calculating the median of K of the neighboring pixels, which is a representative measure for signal changes on a scale larger than one pixel.

$$K_{\text{median}}[r_{\text{img}}, c_{\text{img}}, f] = \text{median} \{ K[r_{\text{img}} - \Delta r : r_{\text{img}} + \Delta r, c_{\text{img}} - \Delta c : c_{\text{img}} + \Delta c, f] \}, \quad (371)$$

where Δr and Δc are the half-widths of the median filter in row and column directions, respectively. Of course, the original pixel ($r_{\text{img}}, c_{\text{img}}$) is excluded from the calculation of the median to make the calculation of the median completely independent of the pixel itself. Since this algorithm operates on image pixels while the source of the transient signal is at the detector, Δr is adjusted according to the binning factor.

Having calculated K and K_{median} , the relative spikeness $k[r_{\text{img}}, c_{\text{img}}]$ of the signal of pixel ($r_{\text{img}}, c_{\text{img}}$) with respect to its neighbors can be expressed as

$$k[r_{\text{img}}, c_{\text{img}}, f] = \frac{K[r_{\text{img}}, c_{\text{img}}, f]}{K_{\text{median}}[r_{\text{img}}, c_{\text{img}}, f]} - 1. \quad (372)$$

Note that when the neighboring pixels have undergone the same time behavior as the pixel under investigation, that is $K = K_{\text{median}}$, k becomes 0 as expected. k is only large when the signal of pixel ($r_{\text{img}}, c_{\text{img}}$) has increased while at the same time the median of the neighboring pixels has not. This corresponds with the second property of transient signals. Pixels can now be flagged transient when the SNR is sufficiently high and k exceeds a certain threshold that depends on several parameters. We will elaborate on that.

Suppose the detector receives light with constant flux f . A transient signal consisting of D electrons is dumped on one pixel \mathbf{x}_{det} between two frame transfers. Ignoring offsets and nonlinearity, we have $S_{\text{trans}}[\mathbf{x}_{\text{det}}] = f \cdot t_{\text{exp}} + D$. Suppose that neighboring pixels receive the same flux and that the flux is constant in time. Then, in the forward sense, binning with unaffected pixels gives

$S_{\text{trans}}[\mathbf{x}_{\text{img}}] = n_{\text{bin}} \cdot f \cdot t_{\text{exp}} + D$. Finally, co-adding with unaffected frames leads to a signal $S_{\text{trans}}[\mathbf{x}_{\text{img}}] = N_{\text{coadd}} \cdot n_{\text{bin}} \cdot f \cdot t_{\text{exp}} + D$ to be read out. After that, in the L01b Processor, correction for co-addition and binning give the following signal at the start of the transient pixel flagging algorithm: $S_{\text{trans}}[\mathbf{x}_{\text{img}}] = f \cdot t_{\text{exp}} + D / (N_{\text{coadd}} \cdot n_{\text{bin}})$.

The transient algorithm, as described above, gives $K[r_{\text{img}}, c_{\text{img}}, f] = 1 + D / (N_{\text{coadd}} \cdot n_{\text{bin}} \cdot f \cdot t_{\text{exp}})$ and the spikeness $k[r_{\text{img}}, c_{\text{img}}, f] = D / (N_{\text{coadd}} \cdot n_{\text{bin}} \cdot f \cdot t_{\text{exp}})$.

Now we can conclude the following:

- Because we want to avoid very low or high signals during corrections, the signal $f \cdot t_{\text{exp}}$, measured in electrons, can for a given short time interval be considered constant. Therefore, the threshold is to be divided by $n_{\text{bin}} \cdot N_{\text{coadd}}$: dilution of a transient spike by co-addition and/or binning is then properly accounted for.
- While the integration time is preferably constant, a change in exposure time during an orbit (while keeping the product $N_{\text{coadd}} \cdot t_{\text{exp}}$ the same) will disturb the algorithm computation. There are, however, only a few of these ICID-changes in an orbit.
- During dark measurements, signals will be low and more or less constant. The detection of a transient signal is then easy; the filter in spatial (swath) direction may be unnecessary.

29.5.2 Remarks

The following remarks are to be made with respect to the transient detection algorithm:

The calculation of S_{median} makes use of the neighboring pixels. It is recommended to have the median width in the wavelength direction larger than the median width in the swath direction for the following reason: If the scenery indeed contains an object that created the sudden increase in the amount of signal, this will certainly be observed over a larger wavelength band. However, the spatial extent of the object will probably not extend over several tens of kilometers (recall that a single pixel observes an area of $7 \text{ km} \times 7 \text{ km}$).

Moreover, we can even argue that that we should not use a filter in the swath direction at all because each row observes a different scene (for example highly reflective clouds), introducing features that will be mistakenly identified as transients.

If it is believed that a transient signal will slightly influence the next measurement (i.e. assumption 1 is not true), the control parameter α can be chosen higher than 0.5 making the weight of the next measurement less, while increasing the weight of the previous measurement.

If in case of saturation of a transient pixel neighboring pixels are affected, we can add a flag for these neighboring pixels.

29.6 Saturation

In case of high signals or improper instrument configuration, saturation of the signal may occur. This can occur in several places:

- ADC saturation (for CCD and CMOS detectors)
- Pixel full-well saturation (for CCD and CMOS detectors)
- Register full-well saturation (for CCD detectors)

If a pixel is flagged for any of these reasons, it will not be used in calculations. However, it will be used in subsequent correction algorithms in the L01b Processor, even though the eventual computed radiance or irradiance is not useful for scientific purposes.

ADC saturation occurs if the signal is such that it overflows the ADC. This is checked on-board for each co-addition separately. If ADC saturation is detected for a single co-addition, the combined co-added signal is set to a special value in the Level-0 data. If the L01b Processor finds such a special value, it flags the pertinent pixel as saturated.

Pixel full-well saturation occurs if an individual CMOS or CCD detector pixel holds too many electrons. Since the excess signal may spill over into adjacent pixels ('blooming' or 'cross-talk'), this not only makes the signal data of the saturated pixel unreliable, but potentially also the surrounding pixels. For unbinned and unco-added images, pixel full-well saturation can be detected by comparing the observed signal with the known pixel full-well value. For binned and/or co-added images, the signals for individual detector pixels are lost, so that in this case, pixel full-well saturation of a single detector pixel may go unnoticed if the detector pixels with which it is binned or co-added together are not saturated. Therefore, pixel full-well saturation of the combined image pixel can only be detected if most of the constituent detector pixels are saturated, although data from the small-pixel column may provide some more information on saturation of individual binned detector pixels.

Register full-well saturation occurs if a CCD read-out register pixel holds too many electrons. This may occur without pixel full-well saturation if the binning factor is high enough. Conversely, in the case with pixel full-well saturation and low binning factor, the register will not be saturated. Register full-well saturation is detected by comparing the observed signal with the known register full-well value.

29.7 Sun glint

When the spacecraft is crossing the equator and the local time is near noon, sun glint can occur above water when the sky is clear and the Sun is near ground pixel zenith. When these conditions occur, the surface reflectivity is increased, due to increasing specular reflection of sunlight by the sea surface. This effect is depicted in Figure 70, which shows the sun glint's effect on OMI data as a grey stripe in the middle of the swath.

Since sun glint may adversely affect Level-2 retrievals, the TROPOMI L01b Processor flags the ground pixels that are potentially affected by sun glint. Now, the extent of the area that is affected by sun glint and the magnitude of the effect depend on the smoothness of the (sea) surface. As this smoothness is unknown to the

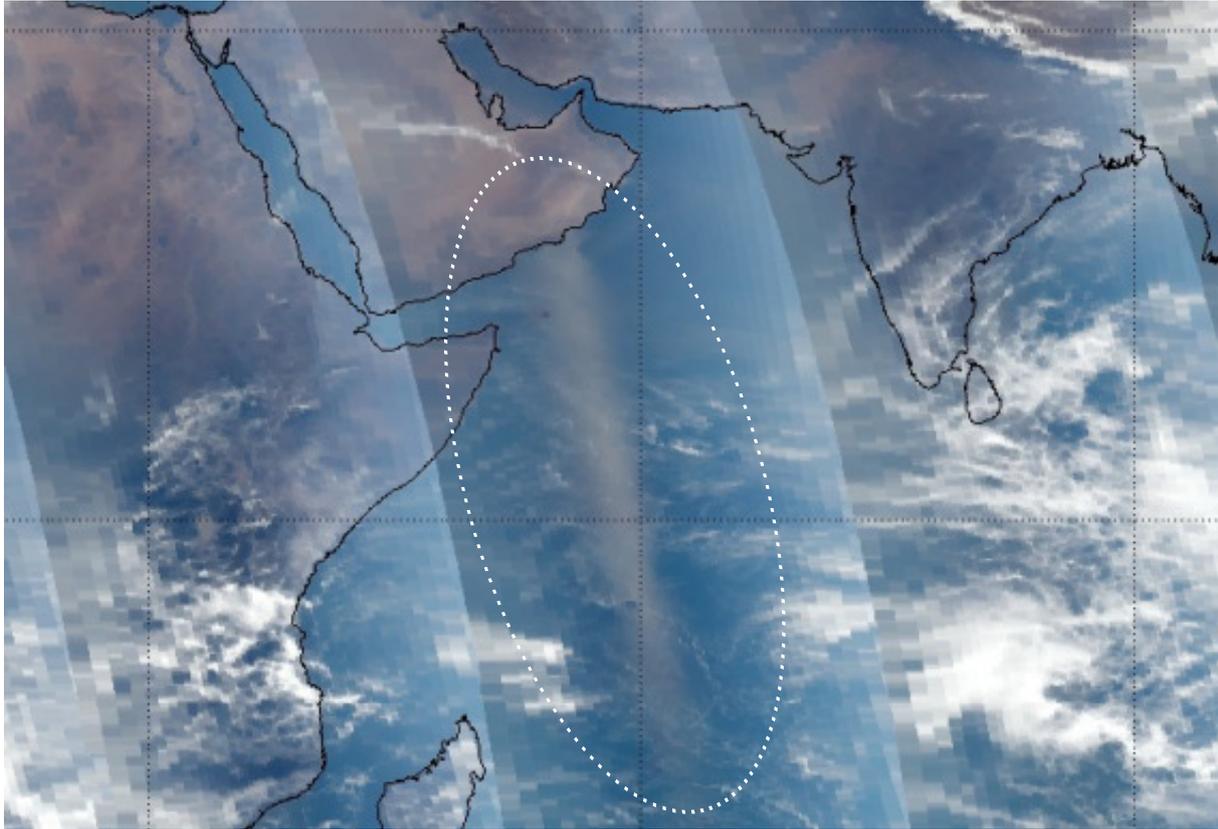


Figure 70: False-color image of OMI data collected on 29 March 2005, showing the sun glint off the coast of the Arabian peninsula. The area where sun glint occurs is indicated by a dotted line.

L01b Processor, the sun glint flagging algorithm uses a static criterion, namely that the sun glint flag is raised if the scattering angle Θ is less than a threshold angle Θ_{\max} :

$$\Theta = \arccos[\cos \theta \cos \theta_0 - \sin \theta \sin \theta_0 \cos(\phi_0 - \phi)] \leq \Theta_{\max} , \quad (373)$$

in which θ_0 and θ are the zenith angles ($= \pi/2 - \varepsilon$) of the Sun and spacecraft, as seen from the ground pixel, respectively, while ϕ_0 and ϕ stand for the azimuth angle of the Sun and spacecraft, as seen from the ground pixel, respectively. Note that this criterion does not discriminate between ground pixels over land and those over water.

The value of Θ_{\max} , based on TOMS, is 30 degrees. Although lower values have been used, e.g. in Sciamachy and GOME-2, the former choice will be the baseline until new information forces us to reassess this decision.

29.8 South Atlantic Anomaly

One source of high amounts of radiation near Earth are trapped particles (protons, electrons) in the Earth's magnetic field. These particles are concentrated in two large belts around the Earth, called the Van Allen radiation belts, see Figure 71. Due to the offset and tilt of the magnetic axis with respect to rotational axis of the Earth, one region of the inner belt causes high levels of radiation very close to the Earth. This region is called the South Atlantic Anomaly (SAA), and is illustrated in Figure 72. The SAA is also visualized in Figure 73, around Sentinel-5p/TROPOMI's altitude.

29.8.1 Point-in-polygon problem

As the SAA is defined by a series of latitude and longitude coordinates at a certain altitude, and thus a polygon, one needs to determine whether the spacecraft resides within this polygon or not. Therefore, the latitude and longitude of the spacecraft's position are tested against this polygon.

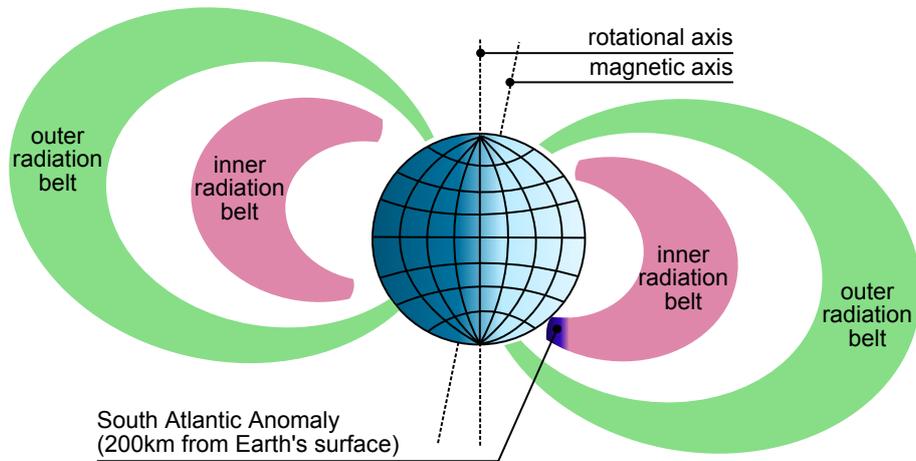


Figure 71: Indication of the location and size of the Van Allen radiation belts, the location of the South Atlantic Anomaly (SAA), and the difference in magnetic and rotational axes of the Earth.

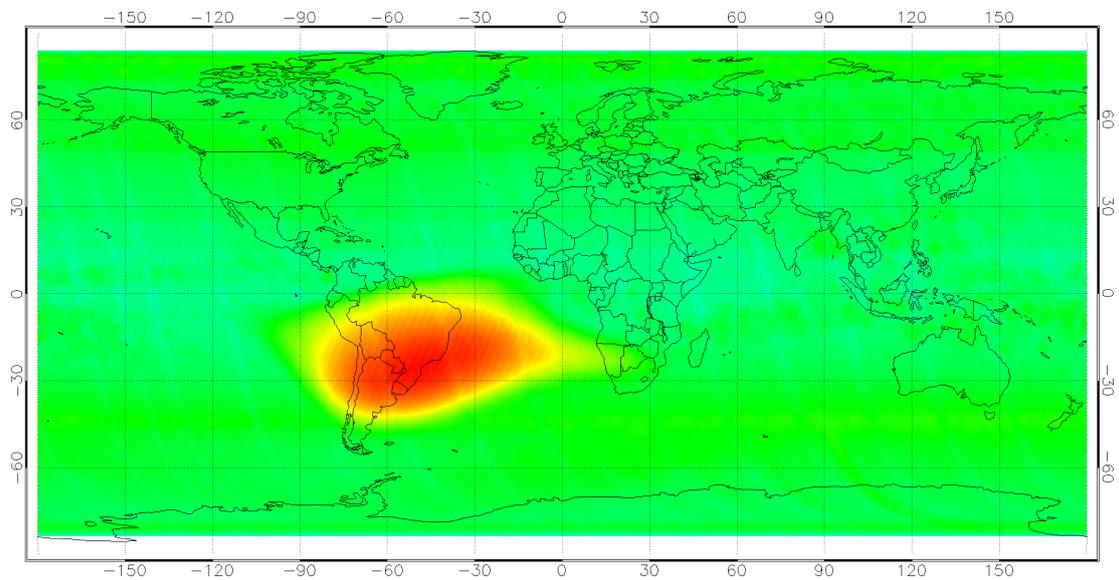


Figure 72: Transient signals density as measured by the OMI instrument onboard NASA's AURA satellite. The plot is the aggregate of one year of data measured at an altitude of 700 km.

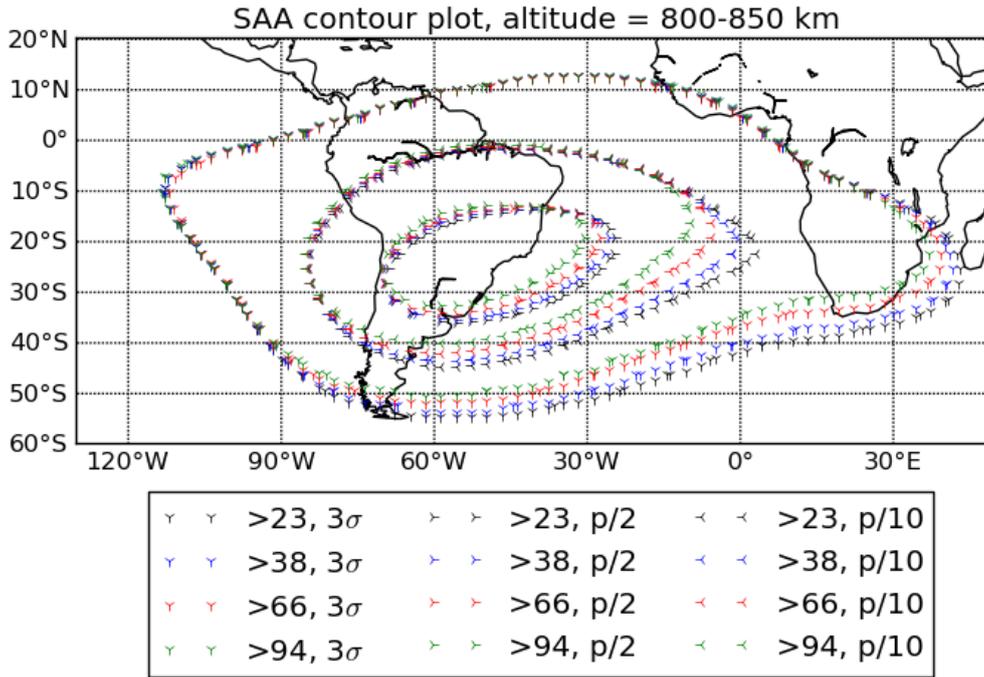


Figure 73: Contour plots of the South Atlantic Anomaly (SAA) for 800-850 km altitude, which is around the S5p/TROPOMI nominal altitude of 824 km. The numbers indicate the limiting proton energies in MeV, while p stands for peak value. '>23, p/10' thus means a contour for proton energy levels higher than 23 MeV, while the area is defined by energy values higher than the peak value divided by ten.

Let us call the spacecraft's coordinates (ϑ_s, δ_s) and that of a polygon point (ϑ_i, δ_i) with i ranging from 0 to n , the number of polygon points. The polygon is drawn by connecting each following point in order of n . The angle α_i that a polygon point i makes with the standard angle reference (eastwards vector) as seen from the spacecraft can be determined by

$$\alpha_i = \arctan 2((\delta_i - \delta_s), (\vartheta_i - \vartheta_s)), \quad (374)$$

which results in a range of $-\pi < \alpha_i < \pi$, which is converted to the range $0 < \alpha_i < 2\pi$. The angle $\Delta\alpha_i$ between two polygon points, α_i and α_{i+1} can then be calculated as

$$\Delta\alpha_i = \alpha_{i+1} - \alpha_i, \quad (375)$$

which is converted to the range $-\pi < \Delta\alpha_i < \pi$. Then adding all polygon angles together results in

$$\alpha = \sum_{i=0}^n \Delta\alpha_i = \sum_{i=0}^n [\arctan 2((\delta_{i+1} - \delta_s), (\vartheta_{i+1} - \vartheta_s)) - \arctan 2((\delta_i - \delta_s), (\vartheta_i - \vartheta_s))], \quad (376)$$

Dividing this angle by 2π results in the *winding number* of the position of the spacecraft with respect to the SAA polygon. If the winding number equals 0, the spacecraft is outside of the SAA polygon, if it equals 1, the spacecraft is inside of the SAA polygon. This theory can be safely applied as the SAA does not cross any dateline or pole boundary.

29.9 Solar eclipses

During a solar eclipse, the TROPOMI instrument might receive less reflected sunlight from certain areas on the surface of the Earth than when there would be no eclipse. As an example, Figure 74 shows the area on the Earth that will be in the shadow of the Moon during the total solar eclipse of 21 August 2017.

Since solar eclipses may affect Level-2 retrievals, the L01b Processor flags ground pixels that reside within the umbra (total eclipse) or antumbra (annular eclipse) or penumbra (partial eclipse) of an eclipse. See Figure 75 for an illustration of the difference between these three types of shadow. The eclipse begins and ends when the penumbral shadow makes first, and last contact with the Earth's shadow, respectively. The eclipse period is defined as the time between these two points.

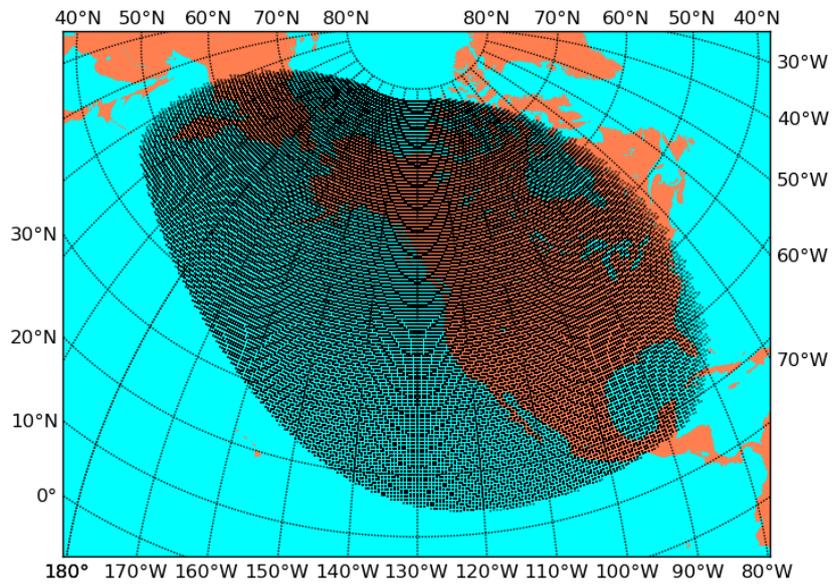


Figure 74: Penumbral shadow cast on the Earth's surface due to the solar eclipse by the Moon on the 23rd of October 2014 during the total eclipse period, as calculated with algorithms implemented in the L01b processor.

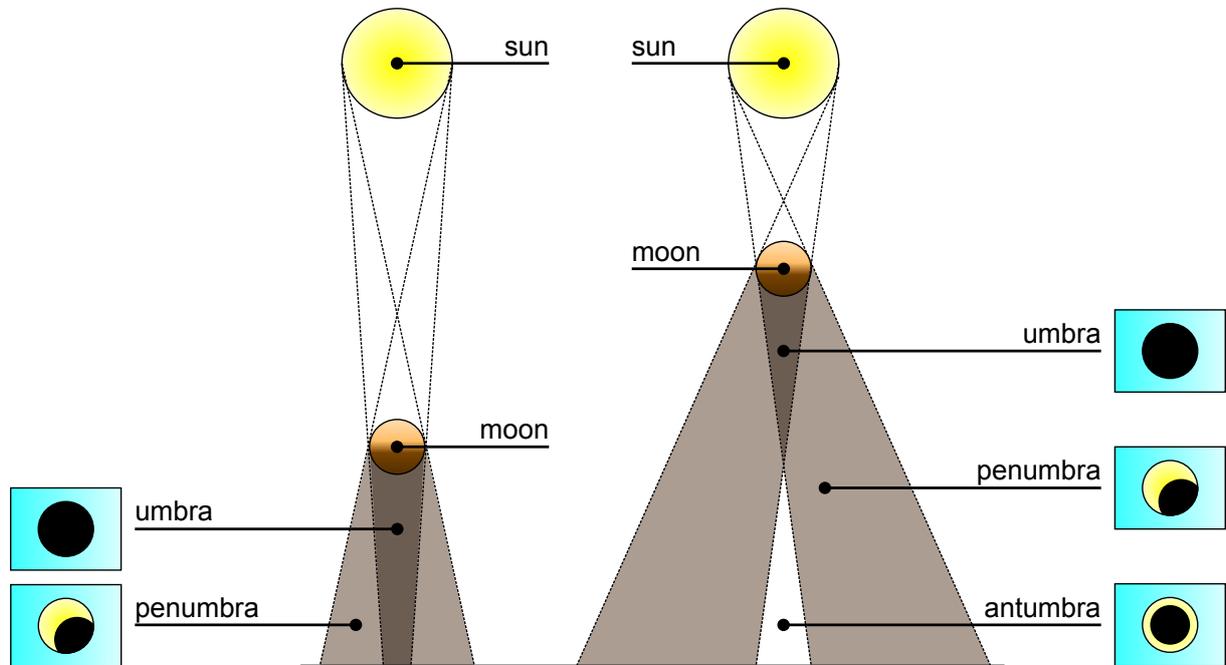


Figure 75: Definition of solar eclipse umbra (total eclipse), antumbra (annular eclipse) and penumbra (partial eclipse).

29.9.1 Eclipse geometry

The full geometry of a solar eclipse at a certain time instance can be described by a set of just 8 parameters: the Besselian elements, as explained in [RD17]. Six of these elements change rather smoothly with time, and can be described accurately with a low-order polynomial expression for the duration of the eclipse. The other two stay practically constant during one eclipse. Table 17 lists the Besselian elements with their symbol, description and unit. Some of the Besselian elements, which were not yet defined in Section 26.2.10, are illustrated in Figure 76.

The Besselian elements can be retrieved from NASA's solar eclipse website (currently [ER23], click on the gamma value of a certain eclipse) as third-order polynomials (with four coefficients c_n), and are evaluated at time t_1 as

$$b = \sum_{n=0}^3 c_n t^n, \quad (377)$$

in which b is any Besselian element and t is obtained from

$$t = t_1 - t_0, \quad (378)$$

by using the Besselian reference time t_0 . All times here are in decimal hours (like a day consists of 24.0 hours).

Table 17: The symbol, description and unit of the Besselian elements, which describe the geometry of a solar eclipse at a certain time instance. The unit for distance is the Earth's equatorial radius a .

symbol	description	unit
x	x-position of the shadow's axis in the fundamental plane.	a
y	y-position of the shadow's axis in the fundamental plane.	a
d	Declination of the shadow's axis from the equator plane.	deg
l_1	Radius of the penumbral shadow circle on the fundamental plane.	a
l_2	Radius of the (ant)umbral shadow circle on the fundamental plane.	a
μ	Greenwich Hour Angle of the shadow's axis in the equator plane.	deg
f_1	Penumbral vertex angle of the shadow's axis.	deg
f_2	(Ant)umbral vertex angle of the shadow's axis.	deg

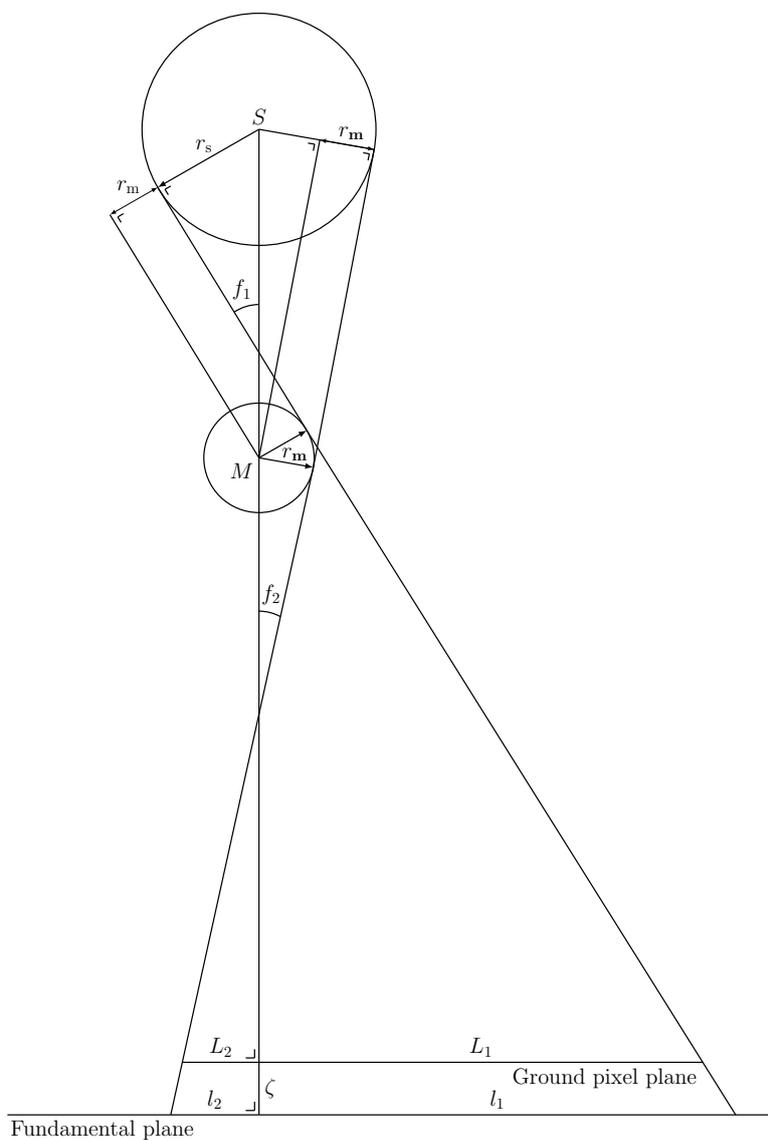


Figure 76: Definition of solar eclipse geometry parameters. Only l , L , f and ζ are used in the equations. When l_2 is negative, it defines an umbra, when it is positive, an antumbra. The latter is shown here. l_1 is always positive.

29.9.2 Eclipse period

From the Besselian elements, the eclipse period can be derived. For an eclipse shadow to fall on the surface of the Earth, the following condition must be fulfilled

$$\sqrt{x^2 + y^2} - l_1 < 1, \quad (379)$$

that is, the distance of the shadow axis to the center of the Earth minus the penumbral shadow radius on the fundamental plane must be larger than 1 equatorial radius of the Earth. Thus, when

$$\sqrt{x^2 + y^2} > l_1 + 1, \quad (380)$$

there is no eclipse shadow on the surface of the Earth, and when

$$\sqrt{x^2 + y^2} = l_1 + 1, \quad (381)$$

the penumbral shadow of the eclipse is just starting or stopping to touch the Earth.

t_0 is always given as a whole decimal hour close to the point of greatest eclipse, and no eclipse lasts longer than six hours. The second equation can be tested numerically for a range of t , say $[-4.0, +4.0]$, with a small stepsize Δt , and for each time t the polynomial expression is evaluated for the Besselian elements x , y and l_1 . Starting at 0 and then both increasing and decreasing t , when the second equation is fulfilled, the time t respectively describes the beginning or the end of the eclipse. The accuracy depends on the size of the stepsize Δt .

29.9.3 Solar eclipse flagging

First, a check will be performed to determine if the measurement time lies within any of the eclipse periods until 2040. This is done by adding the start and stop decimals hour of the day t of the eclipse period to the beginning of the Julian Day (TT) of the point of greatest eclipse, which is given with the Besselian elements, and converting to Julian Days since J2000 (TT). Furthermore, the measurement time is also converted to JD since J2000 (TT), after which they can be quantitatively compared. If the measurement time does not lie within any of the eclipse periods, the algorithm is exited and none of the ground pixels are flagged for this measurement.

If the measurement time does lie within an eclipse period, then for all ground pixels of this measurement it is checked whether or not any of its corner points lie in a penumbral, antumbral or umbral eclipse shadow at the measurement time. To this end the measurement time is converted to t_1 and then to t by making use of the Besselian reference time t_0 .

For the eclipse at hand, all Besselian elements are evaluated with the polynomial expression. All geodetic corner points belonging to a ground pixel position, which was determined in Section 27.1.1, are converted to geocentric Cartesian coordinates as described in Section 26.2.6, after which they are transformed to the Fundamental reference frame by making use of Section 26.2.10 and the evaluated Besselian elements.

Then, as can be seen in Figure 76, the correct radius of the eclipse penumbral and L_1 ant(umbral) L_2 shadow are determined at the height of the ground pixel corner point above the fundamental plane as

$$L_1 = l_1 - \zeta \tan f_1 \quad (382)$$

$$L_2 = l_2 - \zeta \tan f_2, \quad (383)$$

in which ζ is the z-coordinate of the ground pixel corner point in the Fundamental reference frame. L_2 is negative for an umbral shadow, and positive for an antumbral shadow.

The distance D of the ground pixel corner point to the shadow axis is determined as

$$D = \sqrt{x^2 + y^2}. \quad (384)$$

Then, a series of tests is performed for the corner points:

- If ζ is smaller than 0, the corner point lies on the far (night) side of the Earth with respect to the Sun, and can thus not be in an eclipse shadow.
- If l_2 is negative, and $0 \leq D \leq |L_2|$, the corner point is in the umbral shadow of the eclipse.
- If l_2 is positive, and $0 \leq D \leq L_2$, the corner point is in the antumbral shadow of the eclipse.
- If $|L_2| < D \leq L_1$, the corner point is in the penumbral shadow of the eclipse.
- If any of the ground pixel corner points are in any of the three shadow's of the solar eclipse, flag the ground pixel.

29.10 Spacecraft maneuvers

When the spacecraft is maneuvering, the measurements will be disturbed due to the swath deviating from its usual course. Therefore, the instrument will be put into idle mode when this is the case. However, in the event that measurements are still performed while maneuvering, the maneuver flag is raised for these measurements.

This maneuver flag is based on the local normal pointing (LNP) operation mode of the spacecraft, which means that the on-board attitude control system will constantly try to point the spacecraft with the boresight towards the SSP. The nadir point of the spacecraft (the intersection of the boresight with the Earth's surface) will be kept within certain limits of proximity to the SSP. When the spacecraft is maneuvering, the attitude will no longer be in LNP mode, so this can be tested by checking the distance between the nadir point of the spacecraft and the SSP ($d_{SSP-nadir}$). If this distance is larger than the attitude offset threshold maneuver distance $d_{man,thr}$, the spacecraft is said to be maneuvering and the maneuver flag is raised.

First, the nadir point is determined at the measurement time instance. That is, the intersection of the Z -axis (boresight) of the payload reference frame with the surface of the Earth is calculated, resulting in a nadir longitude ϑ_{nadir} and latitude δ_{nadir} . This is done analogous to the ground pixel determination of Section 27.1, using the line of sight that travels along the boresight which has an elevation and azimuth angle of 0 degrees.

The distance $d_{SSP-nadir}$ between the nadir point of the spacecraft and the SSP is calculated with the haversine formula as

$$a = \sin^2\left(\frac{\delta_{nadir} - \delta_{SSP}}{2}\right) + \sin^2\left(\frac{\vartheta_{nadir} - \vartheta_{SSP}}{2}\right) \cos(\delta_{SSP}) \cos(\delta_{nadir}), \quad (385a)$$

$$c = 2 \arctan 2(\sqrt{a}, \sqrt{1-a}), \quad (385b)$$

$$d_{SSP-nadir} = R_e c, \quad (385c)$$

where R_e is the equatorial radius of the Earth. This is an approximation of the distance, by simplifying the problem using a sphere instead of the ellipsoid. A maximum error of 0.3% is now made around the poles, but this is considered small enough compared to the chosen threshold distance.

Part VII

Appendix

A Chebyshev polynomials for curve fitting

A.1 Introduction

In the L01b Processor, it is often necessary to describe a relation between two quantities. This relation is generally acquired by measurements. The relation can be stored using a table, but this is either expensive or involves additional linear interpolation. A more popular method is to describe the relation using a curve that can be mathematically expressed using a number of coefficients. Often, a polynomial function is used:

$$f(x) = \sum_{i=0}^n c_i x^i . \quad (386)$$

Here n is called the *order* or *degree* of the polynomial. c_n is called the leading coefficient and should be non-zero. The term $c_n x^n$ is called the leading term. A polynomial of order $n = 0$ is a constant function; a polynomial of order $n = 1$ denotes a straight line.

The idea now is that only the coefficients need to be stored. The evaluation of the function for a certain value of x is straightforward and should not cost much computational time. It must be checked, however, that x is inside the predefined interval $[a, b]$ where the approximation holds. Extrapolation outside this interval may give hugely erroneous results.

In practice, we do not start from the function $f(x)$ but from two data sets \bar{x} and \bar{y} , where $\bar{y} \approx f(\bar{x})$. We would then like to have a polynomial that resembles the best possible *fit* of \bar{y} to \bar{x} . A polynomial $f_n(x)$ of order n will potentially give a more accurate approximation than a polynomial with a lower order. It is tempting to generate approximating ('fitting') functions of large orders. This, however, has several drawbacks:

- The computational effort involved in computing a fitting function increases significantly if the number of coefficients increases.
- The evaluation takes more time.
- Sometimes the approximation becomes worse if more high-order terms are added. An extreme example is the so-called Runge phenomenon. More often, it turns out that the approximation becomes highly instable near the endpoints of the interval.

We elaborate on the last drawback. The numerical computation of the coefficients involves the solving of a linear system. The numerical properties of the linear system tend to become worse for higher orders, resulting in larger numerical errors. One of the reasons for this instability is the 'similarity' of x^n and x^{n+1} for large n : the monomials x^n and x^{n+1} are very nearly *linearly dependent*, or, in other words, highly *non-orthogonal*. These characterizations can be understood if one looks at the graphs of such functions. We want to express the terms 'dependency' and 'orthogonality' in a more mathematical sense, however.

A.2 Chebyshev polynomials

The approximation of a curve f as described above starts with a set of base functions, in this case polynomials:

$$S_{\text{poly}} = 1, x, x^2, x^3, \dots \quad (387)$$

A linear combination $r_n^S(x) = c_0 + c_1 x + c_2 x^2 + \dots + c_n x^n$ of these base functions is required such that the *least-squares error*

$$M_n^S(f) = \|f - r_n^S\|_2 \quad (388)$$

is minimal. Suppose the curve is described by a list of pairs (x_i, y_i) , $1 \leq i \leq m$. m should be at least $n + 1$. By setting all partial derivatives $\partial M_n^S / \partial a_i = 0$, we get a linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ where \mathbf{A} is a matrix of m rows and $n + 1$ columns with $A(i, j) = x_i^{(j-1)}$; \mathbf{x} is the vector consisting of the $n + 1$ coefficients c_j ; and the right-hand side \mathbf{b} is a vector of size m consisting of the corresponding y_i . It turns out that the matrix \mathbf{A} becomes *ill-conditioned* as n increases. The reason is the following: each column of \mathbf{A} resembles a mapping of the causal data x_i towards one monomial x_i^{j-1} . As we said before, the graphs of these monomials look very similar. That implies

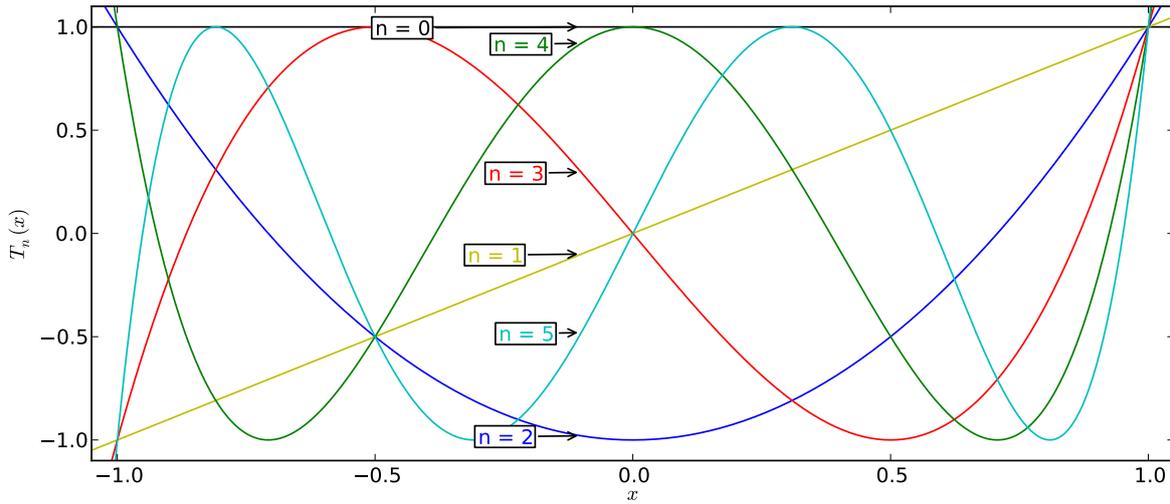


Figure 77: Graph of the first six Chebyshev polynomials.

that solving the system, i.e. inverting **A** directly or indirectly, will cause large numerical errors. Now we go back to the start of this subsection and define another set of base functions:

$$\mathcal{S}_{\text{chebyshev}} = T_0(x), T_1(x), T_2(x), \dots \quad (389)$$

Here T_i is the i^{th} Chebyshev polynomial of the first kind, recursively defined by:

$$T_0(x) = 1, T_1(x) = x \quad (390)$$

and

$$T_{i+1}(x) = 2xT_i(x) - T_{i-1}(x), \quad i \geq 1. \quad (391)$$

Note that there also exist the Chebychev polynomials of the second kind. They are defined by

$$U_0(x) = 1, U_1(x) = 2x \quad (392)$$

and the same relation

$$U_{i+1}(x) = 2xU_i(x) - U_{i-1}(x), \quad i \geq 1. \quad (393)$$

The recursive relation gives

$$T_2(x) = 2x^2 - 1, \quad (394a)$$

$$T_3(x) = 4x^3 - 3x, \quad (394b)$$

et cetera. It is clear that T_i is of order i . These polynomials look quite different from the monomials, see Figure 77. One clue why this is the case is the following: We claim that

$$T_j(x) = \cos(j \arccos x), \quad (395)$$

since

$$T_{j+1}(x) = \cos(j+1)\theta = \cos(j\theta)\cos\theta - \sin(j\theta)\sin\theta, \quad (396a)$$

$$T_{j-1}(x) = \cos(j-1)\theta = \cos(j\theta)\cos\theta + \sin(j\theta)\sin\theta, \quad (396b)$$

and

$$T_{j+1}(x) + T_{j-1}(x) = 2\cos(j\theta)\cos\theta = 2T_j(x)x \quad (396c)$$

which gives the same recurrent relation while T_0 and T_1 are immediately defined from Equation (395).

These polynomials are also special in the following way: in function space, define the inner product of two continuous function f and g as

$$(f, g) = \int_a^b w(x)f(x)g(x)dx, \quad f, g \in C[a, b], w \in C(a, b), \quad (397)$$

Here, $C[a, b]$ is the set of continuous functions on the closed interval $[a, b]$; ‘closed’ means that the endpoints a and b are included. Similarly, $C(a, b)$ is the set of continuous function on the open (i.e. excluding the endpoints) interval (a, b) . The function $w(x)$ is a non-negative weight function.

Now, for the choices $[a, b] = [-1, 1]$ and $w(x) = 1/\sqrt{1-x^2}$, we have for the Chebyshev polynomials:

$$(T_i, T_j) = 0, \quad i \neq j, \quad (398a)$$

$$(T_i, T_j) = \pi/2, \quad i = j, \quad (398b)$$

and

$$(T_0, T_0) = \pi, \quad (399)$$

so all Chebyshev polynomials are orthogonal on $[-1, 1]$.

Without proof we now state that the general least-squares approximation of an arbitrary function $f(x)$ using the set consisting of n Chebyshev polynomials is

$$f_n(x) = \sum_{i=0}^n c_i T_i(x), \quad x \in [-1, 1], \quad (400)$$

where the coefficients c_i are uniquely defined by

$$c_i = \frac{2}{\pi} \int_{-1}^1 \frac{f(x) T_i(x)}{\sqrt{1-x^2}} dx. \quad (401)$$

The integrand may be difficult to compute because of the singularities in -1 and 1 . Therefore we introduce the variable change $x = \cos \theta$ or $\theta = \arccos x$. We use the cosine expression from Equation (395) for the Chebyshev polynomials and get:

$$c_j = \frac{2}{\pi} \int_{\pi}^0 \frac{f(\cos \theta) \cos(j\theta) (-\sin \theta d\theta)}{\sin \theta} = \frac{2}{\pi} \int_0^{\pi} f(\cos \theta) \cos(j\theta) d\theta. \quad (402)$$

This integral can easily be evaluated numerically. It turns out that the coefficients c_j decrease rapidly for increasing j . The error function $f(x) - f_n(x)$ has a particular shape: it oscillates around zero, attaining $n+2$ local extrema (including two boundary extrema) and $n+1$ crossings of the horizontal axis. This oscillation of the error is a direct consequence of the nature of the Chebyshev polynomials.

Hence our preliminary conclusion is that a smooth function can be approximated very well by a Chebyshev polynomial expansion of a certain order, while the coefficients can be computed directly from numerical integration. Of course, this evaluation supposes that the function f is defined everywhere and single-valued; i.e. is a continuous function and preferably often differentiable.

A.2.1 More properties: the derivative

The Chebyshev polynomials have a lot of applications and there are many relations to other special functions. For now, we mention the following properties, related to taking the derivative:

By induction, it can be shown that

$$T_n(x) = \frac{1}{2}(U_n(x) - U_{n-2}(x)) \quad \text{for } n \geq 2. \quad (403)$$

and

$$\frac{d}{dx} T_n(x) = n U_{n-1}(x) \quad \text{for } n \geq 1. \quad (404)$$

Combining Equations (403) and (404) yields

$$2T_n(x) = \frac{1}{n+1} \frac{d}{dx} T_{n+1}(x) - \frac{1}{n-1} \frac{d}{dx} T_{n-1}(x). \quad (405)$$

or

$$\frac{d}{dx} T_{n+1}(x) = 2(n+1)T_n(x) + \frac{n+1}{n-1} \frac{d}{dx} T_{n-1}(x). \quad (406)$$

Suppose we have expressed a function in Chebyshev polynomials: $f(x) = \sum_{j=0}^n c_j T_j(x)$, then

$$\begin{aligned}
 f'(x) &= \sum_{j=1}^n c_j T_j'(x) = c_n T_n'(x) + c_{n-1} T_{n-1}'(x) + c_{n-1} T_{n-1}'(x) + \sum_{j=1}^{n-3} c_j T_j'(x) \\
 &= 2c_n n T_{n-1}(x) + c_{n-1} T_{n-1}'(x) + (c_{n-2} + \frac{n}{n-2} c_n) T_{n-2}'(x) + \sum_{j=1}^{n-3} c_j T_j'(x) \\
 &= 2c_n n T_{n-1}(x) + \sum_{j=1}^{n-1} d_j T_j'(x) \quad \text{where} \quad \begin{cases} d_j = c_j & j \neq n-2 \\ d_{n-2} = c_{n-2} + \frac{n}{n-2} c_n \end{cases} \quad (407)
 \end{aligned}$$

This gives a fast way to compute the derivative of a Chebyshev polynomial expansion in one iteration loop. Note, however, that we can not immediately evaluate the derivative since it is defined for the normalized abscissa. Using the chain rule, we must scale the evaluated answer of a derivative with $2/(x_{\max} - x_{\min})$.

A.2.2 More properties: two-dimensional expansion

In the case of two independent variables x and y , a two-dimensional polynomial expansion can be defined:

$$f(x, y) = \sum_{j=0}^M \sum_{i=0}^j c_{j,i} T_{j-i}(\tilde{x}) T_i(\tilde{y}) \quad (408)$$

Here \tilde{x} and \tilde{y} are normalized variables after linear transformation.

For evaluating this expansion it may be computationally advantageous to write this as a one-dimensional expansion:

$$f(x, y) = \sum_{k=0}^M d_k(\tilde{x}) T_k(\tilde{y}), \quad \text{where} \quad d_k(\tilde{x}) = \sum_{j=0}^{M-k} c_{(j+k),k} T_j(\tilde{x}). \quad (409)$$

This is especially handy if the number of values that \tilde{x} attains is much smaller than the number of values that \tilde{y} will have during evaluation (for example, if x is the exposure time and y a signal value measured in electrons).

Another situation that may occur is when both x and y will be known beforehand but many two-dimensional polynomials exist. This is for example the case when the variables are azimuth and elevation angle; both are constant in an image. Relative irradiance may need to be evaluated for lots of pixels. In that case it is a better idea to compute all combinations $V_{ij} = T_j(\tilde{x}) T_i(\tilde{y})$ beforehand, leaving a linear combination $\sum V_k c_k [\mathbf{x}_{\text{img}}]$ to compute for these pixels.

A.3 Curve fitting revisited

What if the arbitrary function f is not a smooth function, but represented by a discrete data set $[x_i, y_i]$ including noise?

We make the following observations:

- The evaluation of the function is now a problem. There may not be a data point (x_i) near an evaluation point, or there may be more several y_i belonging to identical x_i .
- Alternatively, we can return to the matrix-vector representation as we did before. But this time, knowing about the good properties of Chebyshev polynomials, we use the Chebyshev base instead of the monomial base. We will need a domain transformation first: the causal data x_i has to be mapped towards $[-1, 1]$. This is no problem, once we have established the minimum x_{\min} and maximum x_{\max} of the x_i . Alternatively, we can adjust the x_{\min} and x_{\max} according to our wishes, for instance to remove outliers or allow some extrapolation.

The normalizing mapping is simply

$$x'_i = 2 \frac{x_i - x_{\min}}{x_{\max} - x_{\min}} - 1. \quad (410)$$

That means that the matrix \mathbf{A} will look different except for the first two columns. In fact, \mathbf{A} is (much) better conditioned. The solution of the linear system will have a larger accuracy. Note that the resulting polynomial, after backscaling, should give the same curve approximation independent of the choice of base functions, if we can ignore the numerical inaccuracies.

- The function f will contain noise. We do not want to fit the noise, so we should again be careful not to use too many base functions (i.e. the matrix \mathbf{A} should not contain too many columns). So, on the one hand, we need enough base functions to acquire a good fit; on the other hand, we should still not inflate the order of our approximating polynomial, this time to avoid fitting the noise instead of avoiding numerical instability.

We reassess our first observation. We can as well try to compute the coefficients directly according to Equation (401). In the numerical integration, we should obtain a local (in the sense of being valid in a certain interval) approximation of f in the evaluation points x_j . While doing that we can as well keep track of the local standard deviation.

While the local evaluations of $f(x)$ and its standard deviation $s_{f(x)}$ may not be very accurate, integrating reduces errors so it will provide a good approximation of the coefficients of *both* $f(x)$ and $s_{f(x)}$. This is exactly what we want. We can do this incrementally for increasing order n . Furthermore, we can keep track of the error $f_n - f$ in some norm; if this error does not decrease for larger n , we can assume that we have reached noise levels. Having chosen the optimal order n we solve the related linear system with the Chebyshev polynomials as base functions. Now the accuracy of the coefficients is not merely good, but excellent.

To summarize, our algorithm for curve fitting has become:

1. Transfer the causal data x_i towards the normalized interval $[-1, 1]$.
2. Compute directly, for a range of orders, the Chebyshev coefficients of f and their standard deviations. This already gives a good approximation. Further, insight in the optimal polynomial order n is acquired.
3. Use the set of $n + 1$ Chebyshev base functions for solving the least-squares linear system. The accuracy of the resulting Chebyshev coefficients is excellent.
4. The Chebyshev approximation curve f_n is uniquely given by the set of coefficients and the interval boundaries. Note that evaluation of Chebyshev polynomials is almost as straightforward as evaluation of ordinary polynomials (see below).

In the next section, we will provide a detailed example.

A.4 Example

We simulate a signal based on a function f on the interval $[0, 5]$:

$$f(x) = \arctan(2x - 5), \quad 0 \leq x \leq 5. \quad (411)$$

As we have remarked before, this chosen interval is by no means restrictive since we can always transform an arbitrary interval $[a, b]$ towards the interval $[-1, 1]$. In this particular case, using $t = \frac{2}{5}x - 1$, we get $f(t) = \arctan(5t)$, $-1 \leq t \leq 1$. Besides the necessary condition that Chebyshev polynomials are, for all practical purposes, only defined on the latter interval, computations will numerically be rather accurate since $|t^n| \leq 1$ for all n .

Our data set consists of $m = 400$ evaluations of $f(x)$: $[x_i, f(x_i)]$, $1 \leq i \leq m$. Note that we do not add any noise yet. We approximate the function with four methods:

1. The direct computation of Chebyshev coefficients using Equation (402). This method is tagged *Cheb direct* for usage in Table 18 below. As explained above, it can be expected that this method will provide a very fast way to get a good approximation.
2. The naive, direct linear system solution using ordinary polynomials: *Polyfit*. Because of the non-orthogonality of the basis functions, this method is expected to suffer from numerical instabilities at higher fit orders.
3. An iterative robust method (Levenberg-Marquardt) using ordinary polynomials: *LM fit*. The Levenberg-Marquardt method is a robust method to solve non-linear problems. Although our problem is strictly linear (in the sense that the approximation can be expressed as a linear combination of basis functions), the iterative character of this method means that it will not break down, although the computational cost can become high.

- The direct linear system solution using Chebyshev polynomials: *Cheb fit*. By our choice of these basis functions, we solve a system that is numerically as stable as possible. We do not have to resort to a cumbersome iterative method like Levenberg-Marquardt but can choose a standard method like QR-factorisation or a singular value decomposition. Especially for noisy functions, this method should be superior to the direct computation of Chebyshev coefficients since the noise is taken into account in the least-squares approximation.

In Table 18, the error norm in L_{\max} sense is shown for the four methods. Note that it is also possible to use an L_2 norm, since the norms should be equivalent. Moreover, the computational time required for these methods can be seen.

Order	Error norms				Computational times			
	Cheb direct	Polyfit	LM fit	Cheb fit	Cheb direct	Polyfit	LM fit	Cheb fit
3	0.24904	0.23145	0.23145	0.23145	0.00300	0.00058	0.25712	0.03257
4	0.24904	0.23145	0.23145	0.23145	0.00110	0.00022	0.11010	0.01339
5	0.13597	0.12630	0.12630	0.12630	0.00120	0.00025	0.14497	0.01564
6	0.13597	0.12630	0.12630	0.12630	0.00131	0.00028	0.16733	0.01779
7	0.07725	0.07160	0.07160	0.07160	0.00139	0.00031	0.19954	0.02001
8	0.07725	0.07160	0.07160	0.07160	0.00150	0.00034	0.23372	0.02218
9	0.04503	0.04128	0.04132	0.04132	0.00158	0.00037	0.28213	0.02436
10	0.04503	0.04118	0.04132	0.04132	0.00171	0.00040	0.31224	0.02666
11	0.02675	0.14869	0.02411	0.02411	0.00180	0.00043	0.39326	0.02868
12	0.02675	1.72643	0.02412	0.02411	0.00192	0.00047	2.64219	0.03106
13	0.01612	0.77014	0.02413	0.01455	0.00605	0.00050	0.61538	0.03400
14	0.01612	0.55376	0.01846	0.01455	0.00219	0.00055	1.44428	0.03680
15	0.00983	0.70065	0.02036	0.00888	0.00225	0.00058	1.34475	0.03813
16	0.00983	4.38922	0.01638	0.00888	0.00233	0.00062	3.35150	0.04101
17	0.00605	4.10207	0.01407	0.00546	0.00242	0.00066	2.79580	0.04292
18	0.00605	6.71029	0.01182	0.00546	0.00251	0.00069	3.20646	0.04543

Table 18: Error norms and computational times of different approximation methods. Listed are values for the direct computation of Chebyshev coefficients (Cheb direct), an ordinary polynomial fit (Polyfit), the Levenberg-Marquard method and the using Chebyshev polynomials for the solution (Cheb fit).

The following conclusions can be drawn:

- The error for odd fit orders is the same as the error for the even fit orders immediately following. The reason is that the arctan function is odd; all polynomials of even order do not contribute to the approximation.
- The polyfit method starts to fail from fit order 11 onwards. For all practical purposes, the method breaks down. Numerical instabilities become too large here. Its corresponding graphical behavior can be seen in Figure 78. The 8th-order fit (green) is better than the 4th-order fit (red), but the approximation of even higher order (blue) is far worse. Note that the error is highly tilted to the far end of the graph.
- The LM fit using ordinary polynomials does not break down. Convergence seems to slow at fit orders above 13, however. Moreover, the method demands much computational effort.
- The fit method using Chebyshev polynomials gives good results. It does not take much computational time, although it is an order of magnitude slower than the direct Chebyshev coefficients computation.

Figure 79 shows typical behavior of the approximation for higher orders. The oscillating error is a typical feature of this type of least-squares fitting. Note that there are exactly $n + 1$ extreme values, including the two at the domain boundaries, for a fit of order n . The 'best' error, the so-called minimax error, would be reached if the absolute value of all extreme values would be equal.

Now we move on to the more realistic situation that the signal contains noise:

$$f(x) = \arctan(2x - 5) + N(0, \sigma(x)^2), \quad 0 \leq x \leq 5. \quad (412)$$

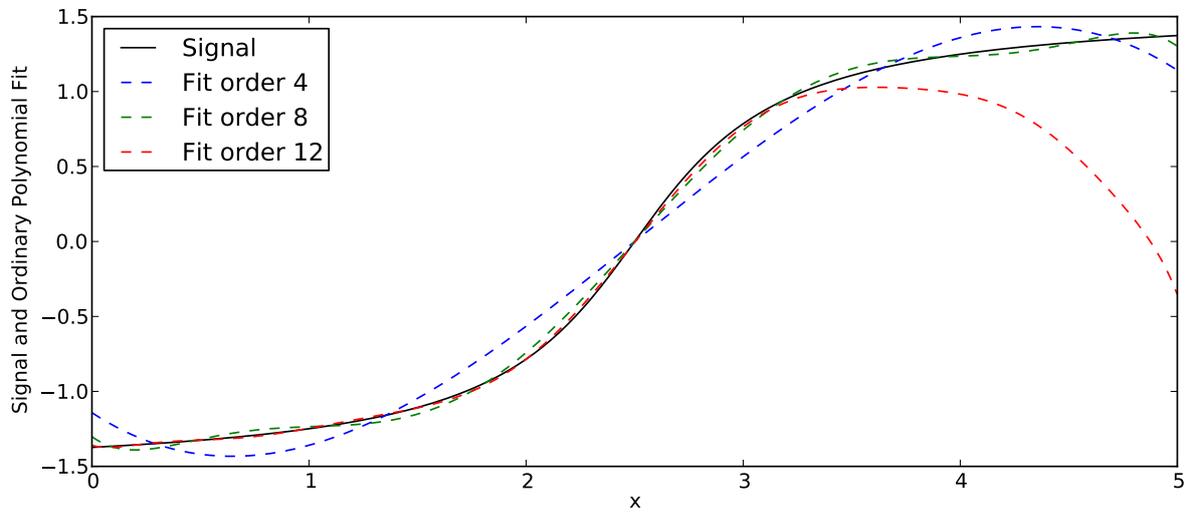


Figure 78: Graph of the approximations of increasing order using the naive polynomial fit.

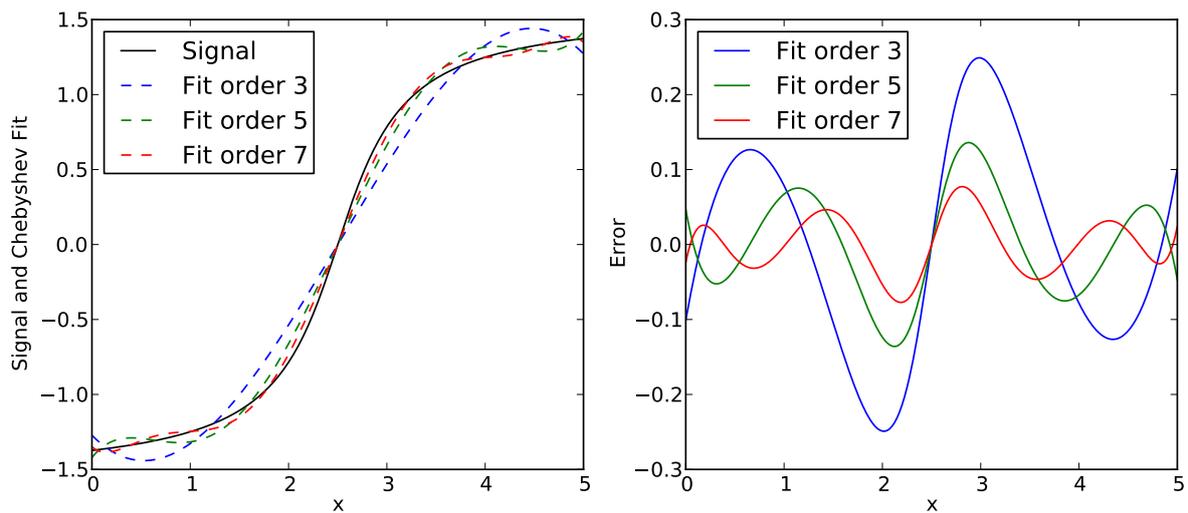


Figure 79: Left: Graph of the approximations of increasing order. Right: The corresponding error graphs.

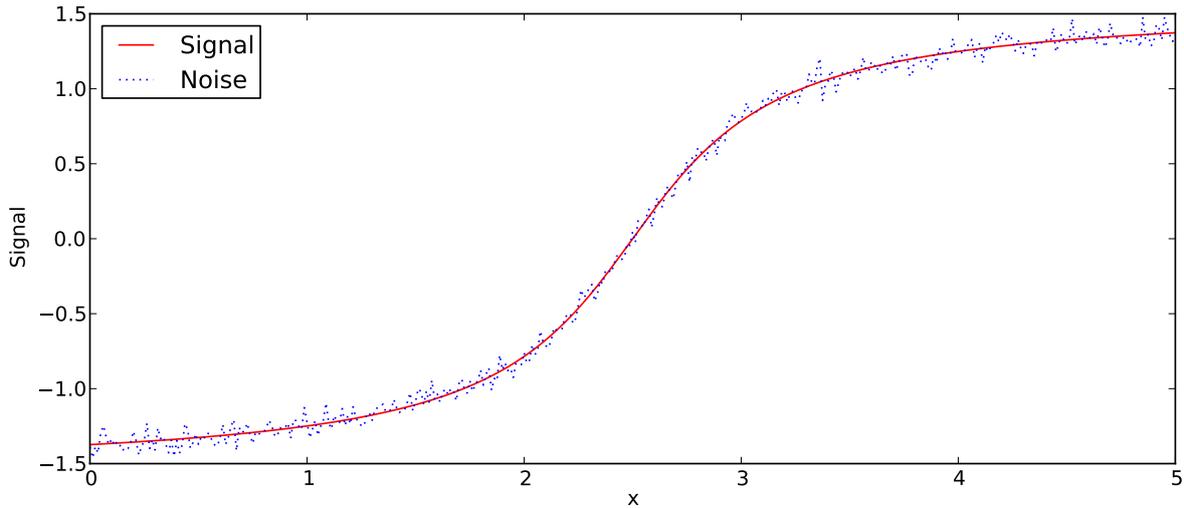


Figure 80: Graph of the noisy signal to be approximated by polynomials.

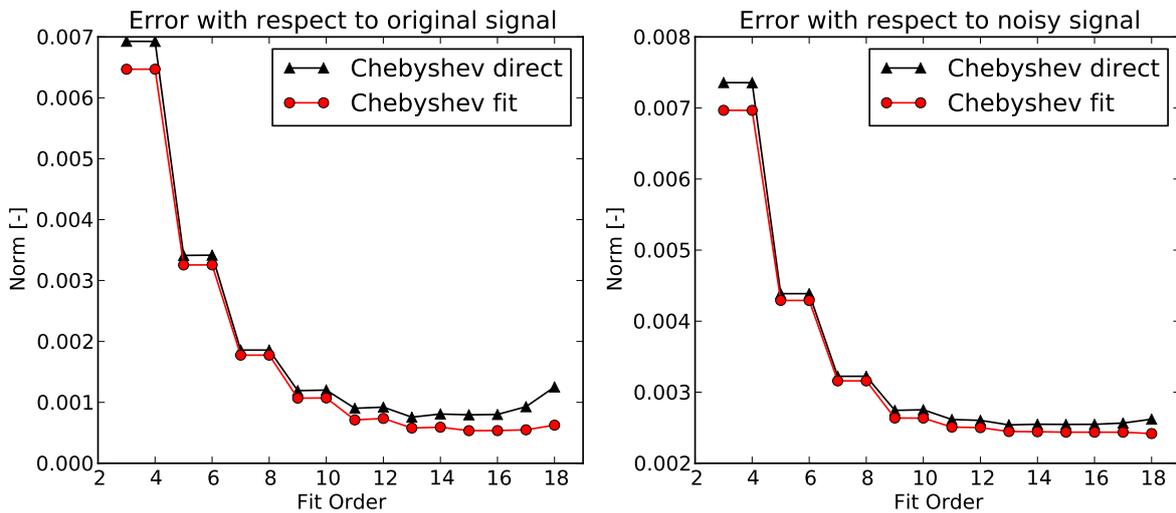


Figure 81: Error as function of fit order with respect to original signal (left) and noisy signal (right).

Where N resembles an normal Gaussian distribution with mean zero and standard deviation σ . In this example, we set $\sigma = 0.05$ for all values of x .

We have to be aware that our assessment of the error should now not depend on the L_{\max} norm anymore, since this would only give an indication of local outliers. This norm and other norms cannot be regarded as equivalent anymore. When we switch to the L_2 norm, we see the following evolution as function of the fit order (see Figure 81). It should be noted that the graph on the left-hand side will in general not be available. However, the behavior of the graphs for the original signal and the measured (noisy) signal behave similarly. Moreover, the fast direct Chebyshev computation behaves in the same way as the least-squares fit using Chebyshev polynomials.

Hence, our strategy is the following: Generate the Chebyshev coefficients using the fast computation method; determine when increasing the order does not yield better results anymore (here for $n \approx 11$); perform a dedicated fit using that order.

With this example, we have given some reasoning concerning the proposed curve fitting algorithm in Section A.3. At the very least, we gain numerical stability and insight in the behavior of the curve and its standard deviation. Moreover, we can be more certain of avoiding the overfitting trap.

B The convolution of the slit function with the solar irradiance spectrum

B.1 How to convolve the solar spectrum with the slit function

We have a tabulated high-resolution solar spectrum: $\{\lambda_i^*, E_i^*\}_{i=0\dots N^*-1}$. We assume that for each wavelength of interest there exists a continuous function $F_{\text{slit}}(x; \lambda)$ describing the slit function, and such that (Section B.2):

$$F_{\text{slit}}(x; \lambda) \equiv 0 \quad \forall x \notin [-\delta_h, \delta_h]. \quad (413)$$

Here δ_h defines a relative wavelength range for which the slit function is measured.

For a given wavelength λ_t we wish to convolve the solar spectrum with the slit function and determine the irradiance $E_{\lambda_t}^*$ measured at that wavelength. We proceed as follows:

- Find the integer p_b such that

$$\lambda_{p_b} \leq \lambda_t - \delta_h < \lambda_t. \quad (414)$$

- Find now p_e such that

$$\lambda_t + \delta_h \leq \lambda_{p_e}. \quad (415)$$

- Calculate

$$\tilde{I}_j \equiv E_j^* \times F_{\text{slit}}(\lambda_j - \lambda_t; \lambda_t), \quad \forall j \in [p_b, p_e]. \quad (416)$$

- Construct now a cubic spline $I_{\text{spline}}(x; \lambda_t)$ from the $\{\tilde{I}_j\}$.

- The sought value is

$$E_{\lambda_t}^* = \int_{-\delta_h}^{\delta_h} I_{\text{spline}}(x; \lambda_t) dx. \quad (417)$$

The L2 developers have provided reference code that performs the convolution and from which the current algorithm has been derived. There are a number of points taken from the reference implementation to consider when implementing the algorithm. These are:

- The integration method should be chosen with care. The reference code we have been given makes use of Gauss integration. The reference code has also been run integration with Simpson's rule using as abscissas the wavelengths $[\lambda_{p_b}, \lambda_{p_e}]$. Using the OMI slit function ($\delta_h = 1.5$ nm, with a sampling interval of 0.01 nm), there are no differences between the two methods.
- The reference code performs piece-wise Gauss integration using at most 13 points per segment taken in the range $[\lambda_{p_b}, \lambda_{p_e}]$.
- When interpolating the tabulated slit function with a cubic spline the reference code checks that Equation (420) hold using $\delta_h = 1.2891456$ instead of the full range. Given that the OMI slit function is 0 outside of this range, this has no effect.

B.2 How to interpolate the slit function

In this section we give an algorithm to interpolate the slit function. The algorithm makes an assumption about the way the slit function is made available in the CKD. The algorithm may have to be modified, should the assumption not longer hold.

We assume that the slit function is available in tabulated form. For each (possibly binned) row in the detector there exists a grid of strictly monotonically increasing wavelengths $\{\lambda_i\}_{i=0\dots N_i-1}$. For each λ_i the corresponding slit function is described by $\{F_{i,s}, \delta_{i,s}\}_{s=0\dots N_s-1}$, where the $\delta_{i,s}$ are wavelength offsets with respect to the central wavelength λ_i . For each instrument it is convenient to make the $\delta_{i,s}$ the same irrespective of wavelength and drop the subscript i . Also, we take the range covered by the offsets symmetric around the central wavelength so that $\delta_s \in [-\delta_h, \delta_h] \forall s$. In summary, the slit function is tabulated as a three-dimensional data set with three dimensions: detector row, reference wavelength, and wavelength offset with respect to the reference wavelength.

Two interpolations are required:

1. The tabulated slit functions are interpolated for an arbitrary $\lambda \in [\lambda_0, \lambda_{N_i-1}]$. This delivers a new tabulated representation of the slit function. This interpolation is done linearly, as explained below.

Consider $\lambda \in [\lambda_0, \lambda_{N_i-1}]$. Find the index p so that $\lambda_{p-1} \leq \lambda \leq \lambda_p$. It is clear that the equal signs cannot hold at the same time because the λ_i are strictly monotonic. Now define

$$a = \frac{\lambda - \lambda_{p-1}}{\lambda_p - \lambda_{p-1}}, \quad (418a)$$

$$b = \frac{\lambda_p - \lambda}{\lambda_p - \lambda_{p-1}}. \quad (418b)$$

The interpolated tabulated slit function is given by

$$F^* = aF_p + bF_{p-1}. \quad (419)$$

2. A tabulated slit function is interpolated $\forall \delta \in [-\delta_h, \delta_h)$. This makes the slit function a continuous function. This interpolation is done by means of a cubic spline. The algorithm must make sure that for the interpolating function, call it F_{spline} , the following holds:

$$\int_{-\delta_h}^{\delta_h} F_{\text{spline}}(t) dt = 1. \quad (420)$$

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