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B. Ording

A. Ludewig

R. Hoogeveen

D. ten Bloemendal

et al.



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RESULTS OF THE TROPOMI CALIBRATION CAMPAIGN

B. Ording¹, A. Ludewig², R. Hoogeveen³, D. ten Bloemendal¹, J. Dingjan¹, R. Voors¹, J. de Vries¹.

¹Airbus Defence and Space, Netherlands. ²Royal Dutch Meteorological Institute (KNMI), Netherlands, ³SRON Netherlands Institute for Space Research.

I. INTRODUCTION

The TROPospheric Monitoring Instrument (TROPOMI) is a sun-backscatter imaging spectrometer. It is the single instrument on board ESA's Copernicus Sentinel-5P satellite, which is now planned for launched in early 2017. TROPOMI will monitor the Earth's air quality and climate by means of accurate UV-VIS-NIR-SWIR spectroscopic measurements of atmospheric constituents like O₃, NO₂, SO₂, CH₄, CO, CH₂O, and aerosol properties. TROPOMI will continue the data series produced by SCIAMACHY [1] and OMI [2], but with much improved spatial resolution and accuracy.

TROPOMI was calibrated in a 125-day 24/7 measurement campaign [3] by a joint effort of industry and science teams. To address the various calibration needs, a large number of distinct Optical Ground Support Equipment (OGSE) were required, which differed in spectral bandwidth (broadband vs. narrowband), angular field size (point/line-like or a few degrees), uniformity, stability, and brightness. Because of the broad spectral range, multiple optical setups were often needed. The OGSE were implemented as reusable modular setups. Calibrating the instrument's spectral response function and stray light properties are particularly challenging and therefore required a multitude of different setups: spectral line sources, gas cells, a broadband point source, an echelle spectrograph, a band-filter setup and two types of tuneable lasers.

II. CALIBRATION INFRASTRUCTURE

TROPOMI was calibrated at its operational temperature in thermal vacuum. The instrument's straight slits result in curved fields of view towards Earth, covering 108° in azimuth and a total of up to 7° in elevation. Therefore a 2-axis rotatable cradle was needed in the vacuum chamber to be able to calibrate the whole field of view. The calibration infrastructure consists of the facility control, the TROPOMI Central Checkout System (CCS) and a storage/processing server. The infrastructure is presented in Fig. 1. The facility control system regulates the pressure, test heaters and the LN₂ flow. The test heaters are placed at the instrument radiator interfaces controlling both the temperature of the facility equipment as the instrument temperature when TROPOMI is switched of. The house keeping data from the facility was only used to assess whether the measurement conditions were nominal.

At the TROPOMI Central Checkout System all systems regarding the measurements can be controlled with both manual commanding of from a script:

- The TROPOMI ICU are controlled via the spacecraft simulator EGSE. From the EGSE the measurement data is routed to the CCS. On the CCS the images are displayed in real-time. Furthermore, the data is sent from the EGSE to the processing server where it is pre-processed immediately for quick analysis during the measurement itself.
- From the 24 different OGSE the tuneable lasers and the scanning slit-function-stimulus are controlled
- TROPOMI was mounted on a 2-axis rotatable cradle in order to scan the whole field of view of the instrument

From the EGSE the data is directly transferred to and processed on-site by the level-1b processor [4]. Together with dedicated quicklook and analysis tools this provides the opportunity to do on-site near real time analysis of the quality of the measurement. Also the level-1b processor is tested in an operational scenario.

During the calibration campaign there is not enough time to complete the Calibration Key Data (CKD) derivation and to assess if the instrument performance meets all requirements. Instead the pre-processor was used to assess the quality of the measurement itself in terms of e.g. signal-to-noise and illumination homogeneity in order to derive the CKD with sufficient accuracy. The capability to perform this quality assessment in parallel with the commissioning of a new measurement setup was a key success driver for completing the calibration campaign within the given timeframe. The calibration key data itself was derived on separate processing infrastructure by off-site personel.

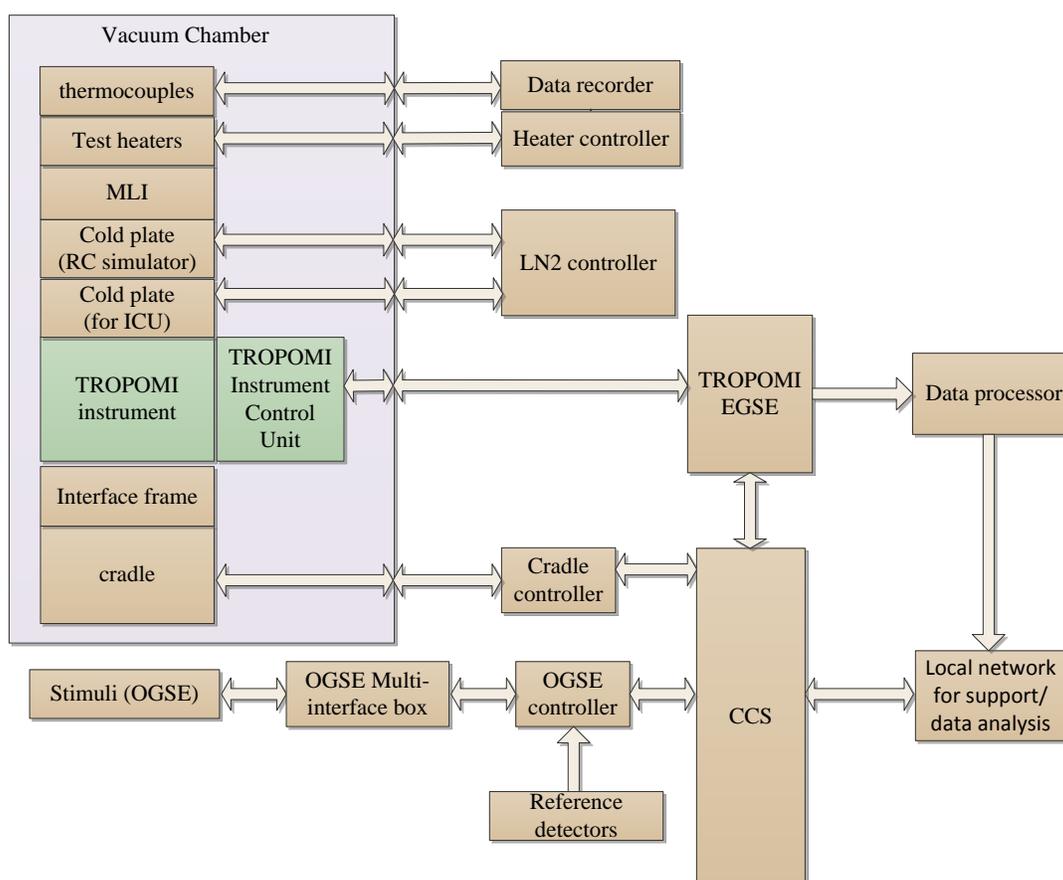


Fig. 1. Schematic overview of the TROPOMI calibration infrastructure

III. DESCRIPTION OF THE OPTICAL SETUPS

A. External Optical Setups

An important driver for the TROPOMI calibration campaign was schedule. Most critical was the time available for the execution of the campaign, closely followed by pre-calibration commissioning of the (O)GSE, and design and development of the 24 individual OGSE. In order to accommodate the tight schedule for the TROPOMI calibration campaign, a modular approach for the OGSE was chosen. Approaching the combined OGSE as a system may not have provided the most optimal configuration for each individual stimulus, but did provide a faster and more structured commissioning phase, and facilitated quick setup changes.

Some of the challenges and boundary conditions for the OGSE were:

- Some of the OGSE was quite late in development and commission
- To maximise the science performance, the calibration campaign duration was to maximum extent stowed with measurements. Maximising the measurement time and minimising “down time” for OGSE change-over was crucial
- The cleanroom containing the TROPOMI calibration vacuum chamber was shared with other projects. Special measures needed to be taken to minimise the cross-influences and cross-dependencies of the various projects.

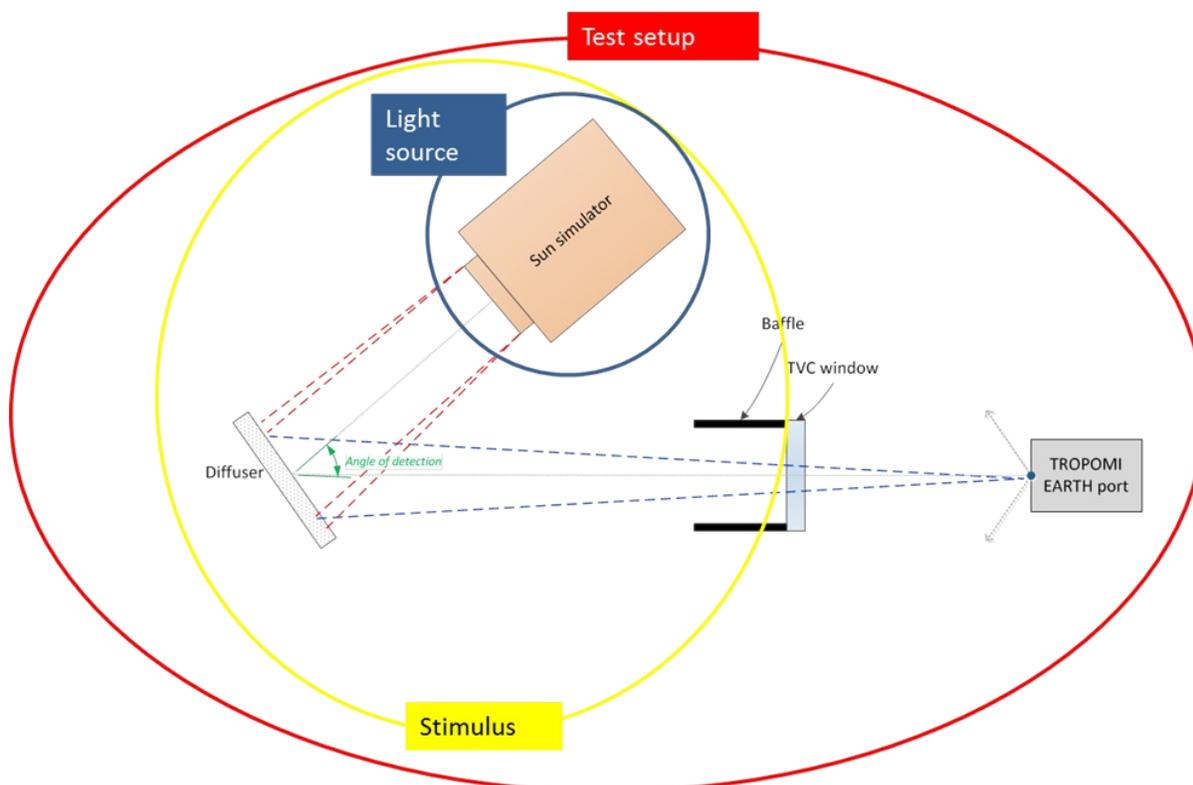


Fig. 2. Schematic example of an OGSE setup

The following solutions were chosen to meet the above:

- Modular approach to OGSE – a relatively small number of source and various optics modules could be combined to form the 24 different OGSE
- Multiple optical tables on semi-kinematic bases – careful planning of the order of measurements and the assignment of stimuli to tables made it possible to commission OGSE while other OGSE was in use for calibration measurements, and for longer-duration OGSE changes to be performed “off-line”, not impact the measurement schedule
- Module alignment during commissioning, with mechanical references enabling removal and sufficiently accurate re-positioning of modules
- A light-tight black enclosure around the optical table, interfacing with a baffle on the vacuum chamber
- Scheduling of calibration measurements using instrument-internal sources during OGSE changeovers
- Very direct and open communication between OGSE engineers, test execution operators, and scientists, who would run instrument quick-look directly after, or even during, OGSE setup

These measures resulted in:

- Quick OGSE changes – most OGSE changes could be performed in less than 8 hours, and in some cases in as few as one or two.
- Very little alignment necessary during calibration execution – cross-checks validated earlier alignments
- Quick modifications on the fly due to feedback from quick-look
- During the 4 months (end-to-end), 24/7 operation calibration campaign, the total overhead / downtime was less than 15%.

Modules from which most of the OGSE could be constructed included one of three collimator modules (either using an off-axis parabola, a 2-lens collimator, or a 3-lens re-imager), one of several field stop modules (various sizes and shapes, pinholes, lines, rectangles, some water cooled, etc), different illumination modules (direct, through an integrating sphere, or through transmission diffusers), and various sources.

During execution, the only alignment that needed to be performed were the location and orientation of TROPOMI, using a laser tracker and theodolites; recording the orientation of the collimator mirror relative to TROPOMI using theodolites (specifically for star stimulus measurements); and the location and orientation of the FEL lamp(s) and/or diffuser(s) for absolute radiometric measurements.

Problems can occur in even the best-planned and prepared campaigns. In our campaign, two more significant issues occurred.

The first was rapid output power degradation of a commercial variable-wavelength pulsed laser. Even with manufacturer technician on-site support and having available a spare laser, the issues were not resolved satisfactorily. By re-organising the measurement schedule and quick iterations with the scientists, a significant portion of the measurements were still performed, but unfortunately not as many and not all with the quality as hoped for.

The second issue was the sun simulator xenon lamp showing at times instability. During commissioning the stability was measured and found adequate, but when the setup was placed in front of the chamber, it deteriorated and could not be used anymore in the end. Fortunately many of the calibration products could also be obtained with measurements from other sources, but some additional work is still needed.

A challenging calibration campaign like this one sometimes leads to somewhat less-conventional approaches. A significant challenge for absolute radiometric measurements with a FEL lamp is the interaction of the FEL lamp with the environment. The accurate and calibrated irradiance generated by the lamp is influenced by indirect light paths (both diffusive and specular) adding to the direct light path, and reflections back onto the filament which can heat the lamp. Therefore, it is best to use the lamp in an open environment without any surfaces nearby. For the radiometric calibration of the Earth-port, the instrument should measure the radiance off a diffuser, irradiated by the FEL lamp, and any direct line of sight between the instrument and the FEL lamp should be blocked by baffles. These baffles should, of course, not direct light towards the diffuser (indirect light paths), nor back to the FEL lamp (heating). To solve this issue, we implemented large flat mirrors between the FEL lamp and the instrument, angled in such a way that the FEL lamp never reflected towards itself, the diffuser, and the instrument.

B. Internal Light Sources

During the calibration campaign internal light sources were used to do repeated series of measurements in order to get 'long term' stability assessment (= 4 months) and detector and electronics settings optimization and characterization and calibration. The advantage of incorporating the use of the internal light sources into the calibration campaign is that these take-up no setup time. Consequently these tests we performed during the change of 'external' setups. This flexible employability of the internal light sources significantly increased the time TROPOMI could do useful calibration measurements.

TROPOMI has 4 types of internal calibration sources:

- Detector LEDs; The LEDs are placed just outside the optics within the spectrometer channels and illuminate the detectors through only a part of the imager optics; delivering a 'flat field' illumination. These LEDs can be used to monitor the non-spectrally depended detector characteristics and the electronics chain.
- A White Light Source (WLS) with a diffuser surface in the calibration unit. The WLS illuminates the whole optical path of the instrument and because it is spectrally broadband over a diffuser surface, illuminates all detectors over all viewing angles. The WLS can be used to determine and monitor the Pixel Response Non Uniformity (PRNU) and check for throughput degradation
- As the WLS itself will also degrade a blue LED is also present in the calibration unit in order to cross-reference the output of the WLS. This LED is an experimental calibration source and has to prove its use in orbit
- In order to monitor the slit function of the SWIR spectrometer, 5 temperature tuned laser diodes are in the calibration unit. By changing its temperature a scan of about 2 nm wide can be made to monitor the SWIR slit function.

IV. TROPOMI CALIBRATION KEY DATA ACCURACY

The requirements on calibration key data parameters measurements were derived from requirements on Level 1b. The actual impact of the L1b accuracy on L2 products can only be assessed in detail once there are radiance measurements available. The accuracy on Level 1b depends on the correction algorithm accuracy, the accuracy of the algorithm to determine the calibration key data, the calibration accuracy of sources and the achieved signal-to-noise ratio of the measurements.

The validation of the calibration of the TROPOMI instrument therefore needs to be manifold: the L01b processor software is validated to provide the correct implementation of the instrument model, the calibration measurements provide validation of the instrument model, the output of the L01b processor is validated against

the requirements, and dedicated validation measurements are used to determine the accuracy and precision of the calibration key data.

The on-ground calibration campaign of TROPOMI was planned such, that for all calibration measurements there were also validation measurement foreseen.

A. Radiance Responsivity

The radiance responsivity of the TROPOMI instrument was determined in two steps: the absolute response was calibrated for a central swath angle with absolute calibrated sources. With a stable but uncalibrated source the entire swath was measured and the relative radiance responsivity was determined.

The accuracy of the relative response was determined by comparing relative measurements performed with an integrating sphere to measurements performed with the absolute sources. The agreement is between 0.6% to 1.2%.

The accuracy on the absolute part of the radiance responsivity was determined by comparing the results for the different combinations of the two calibrated diffuser plates and the two different calibrated FEL lamps. The accuracy of the calibrated sources, the uncertainty on the diffuser-lamp distance and geometrical uncertainties are also taken into account.

The absolute radiance responsivity is calculated as an average of results obtained for different lamps, diffusers, and cradle rotation angles. The accuracy of the absolute radiance responsivity is 2-4% for UV, 2% for UVIS, 1.6% for NIR, and 2-3% for SWIR. The L1b requirement on the absolute radiometric accuracy is 2%. All TROPOMI detectors are below this value when considering uncorrelated errors. For correlated errors band 1 (lower UV range) has an accuracy of 4% and the SWIR detector 3%.

The achieved accuracy reflects discrepancies between the results obtained for the various combinations of lamps and diffusers. A large part of the uncertainty (0.5-1.5%) is attributed to lamp or diffuser calibration uncertainty, the remaining differences are unexplained.

Comparing different subsets of the measurements, for example all lamp-diffuser combinations at a certain distance, results in accuracies of within 1% for all detectors. The pixel-to-pixel uncertainty of the radiance responsivity is relatively small (<0.01%).

B. Irradiance Responsivity

The irradiance responsivity of TROPOMI is split up in the relative sun-angle dependent part and the absolute calibration at a reference angle.

The relative irradiance responsivity calibration measurements failed, as the employed stimulus (sun simulator) showed both large drifts and spikes in its output. This calibration key data will be recovered with in-flight measurements during E1 by moving the instrument platform to the required azimuth angles.

The absolute irradiance responsivity was determined for both internal quasi volume diffusers (QVD) using two calibrated FEL lamps measured at three distances (d1, d2 and d3). The resulting calibration key data was calculated, per QVD, as the average result of both FEL lamps at the shortest distance d1. The roughness of the internal diffuser surfaces causes interference patterns (speckle) that are dependent on the wavelength, viewing angle, and location on the diffuser. They are hard to characterize because of the many factors that influence them, so they are smoothed out. The diffuser features in the SWIR follow a normal distribution with a standard deviation of 0.4% for both QVDs. With the UVN detectors no diffuser features could be observed.

To determine the accuracy of the absolute irradiance responsivity various validation methods were used: measurements were repeated, the measurements at different distances were fitted to the inverse-square-law and the two calibrated FEL lamp results were compared. The different verification methods result in an accuracy better than 1.5%. This is well within the 2% required on Level 1b.

C. Instrument BSDF

The instrument bi-directional scattering function, (BSDF) was initially planned to be determined from measurements using the sun simulator (SUNSIM). This stimulus was however not sufficiently stable for this purpose, resulting in uncertainties from 5% up to 30%. As a backup, measurements with an integrating sphere were performed (SPHERE). These measurements resulted in a too low signal-to-noise ratio for bands 1 and 3. Therefore the instrument BSDF has been derived from measurements with the absolute calibrated FEL lamps and external calibrated diffusers.

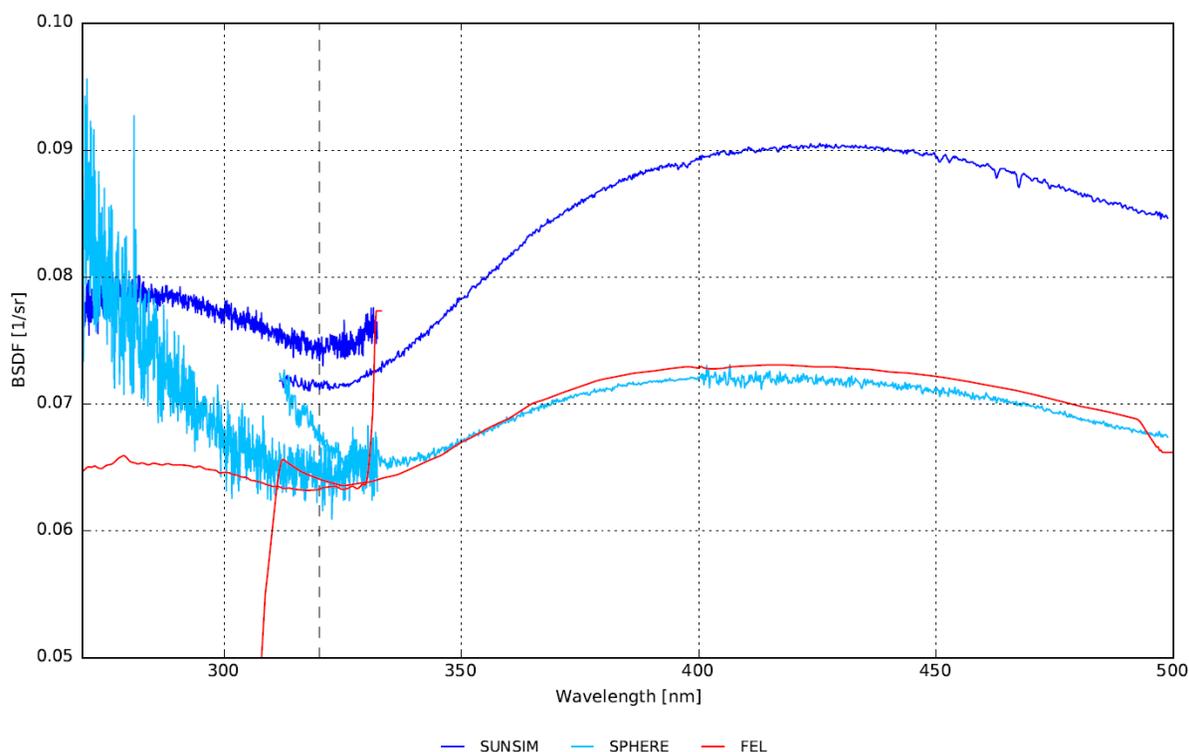


Fig. 3 The FEL-BSDF, SPHERE-BSDF and SUNSIM-BSDF of detector 1 and 2. Figure courtesy of KNMI.

Fig. 3 shows the comparison between the 3 BSDF measurements: The vertical dashed line at 320 nm indicates where the performance range of the UV detector ends and the performance range of the UVIS detector begins. Ideally, the BSDF curves of both detectors should overlap. All BSDF curves are of the optical axis rows. The UV and UVIS channels have a different field of view and therefore the optical axis rows might not follow identical paths through the diffuser. This may account for small differences between detectors 1 and 2.

The accuracy achieved for the BSDF is 4.2% for the UV, 2.2% for the UVIS, 1.7% for the NIR, and 3.4% for the SWIR. These values are higher than the 2% required on Level 1b. The main source for the uncertainty is the calibration of the external diffusers. The instrument BSDF has been validated qualitatively with independent measurements for all detectors.

D. Line-of-sight and Co-registration

The line-of-sight and co-registration were determined with just one stimulus; an independent validation will be performed in-flight using Earth targets such as coastlines. The validation of the analysis of the on-ground measurements was done by comparing direct fitting and fitting through the derived point spread function. The SWIR detector showed some deviation between the two methods, as a warm field stop influenced the line-of-sight fit. The line-of-sight angles are therefore derived from the fitted point-spread-function. A conservative estimate of the error in the calibrated line-of-sight angles results in 100 m (UV), 103 m (UVIS and NIR) and 135m (SWIR) on-ground at nadir for the respective detectors. The accuracy of the parameters stems from alignment accuracies of the stimulus and fit residuals. The inter-band co-registration difference is largest between NIR and SWIR (15-37 km) and smallest between NIR and UVIS (2-15km).

E. UVN Instrument Spectral Response Function

The instrument spectral response function (ISRF) for the UVN detectors has been determined from measurements with two stimuli: the slit function stimulus (for NIR and mainly UVIS) and the tunable laser (mainly for UV and partly UVIS and NIR), and validated using two additional spectral line sources. The analysis included both Sun port and Earth port measurements. The use of two distinct stimuli has enabled cross validation and provided redundancy, which has proven to be essential during the calibration campaign, as laser reliability and signal-to-noise issues for the slit function stimulus reduced the number of usable measurements. The ISRF for the UVN detectors has been determined within the required 1% accuracy. The ISRF measured via the Earth port is within 1% identical with the one determined via the Sun port.

F. SWIR Instrument Spectral Response Function

The SWIR ISRF has been determined by using the external tunable cw laser. The complete SWIR range has been scanned with the laser, both for the Sun port and the Earth port, enabling a comparison. An independent validation was performed by employing the internal lasers, although these lasers scan only a small part of the spectral range. It is found that the ISRF depends on the exact location (spectral and spatial) on the detector. All three methods agree within the 1-2 %, where the larger deviations are most likely due to measurement artifacts.

G. UVN Spectral Calibration

The spectral calibration for the UVN measurements were performed using a combination of spectral line sources and slit function stimulus. The overall uncertainty of the wavelength calibration key data is estimated to be 9pm for the Earth port and 16pm for the Sun port (standard deviation). The comparison of Sun and Earth port spectral calibration shows agreement within 25pm for most of the detector pixels.

The achieved accuracies are not as high as required on Level 1b with 4-8 pm for UV and 2 pm for UVIS and NIR.

H. SWIR Spectral Calibration

The SWIR band exhibits many strong absorption features of methane and CO. The di-atomic CO has a very nice regular absorption spectrum, ideally suited for spectral calibration. A 30 cm gall cel between the white light source and TROPOMI was used with 100 % CO filling. All absorption lines are assigned to known wavelengths of CO and subsequently a 2D fitting routine of all absorption lines on the detector is performed. The accuracy for this procedure is well below 1 pm. Differences between Sun port and Earth port wavelength calibration is less than 5 pm peak-peak. An independent validation using 6 emission lines of a PtCrNeAr emission lamp shows typical offsets of 5 - 10 pm, but these can largely be explained by a 0.1K change in instrument temperature. The spectral smile of the SWIR channel is about half a spectral pixel only.

I. UVN Straylight

The measurements for the straylight correction for the UVN detectors were done with different stimuli: a white light source, a range of band filters covering the entire spectral range, and a laser to measure the straylight contributions close to the main signal.

The straylight correction reduces the average straylight from 2.05% to 0.81% for UV, from 1.23% to 0.53% for UVIS and from 4.04% to 3.31% for NIR, whereas the noise level is of the order of 0.01 %.

The L1b requirements hold on a model straylight scene, the so-called 'hole in the cloud'. This kind of illumination cannot be easily re-produced with a stimulus and was therefore modeled from calibration measurement data.

This model straylight scene shows that the implemented corrections is within requirements for UV and UVIS, whereas NIR shows as much as 10 times more straylight than allowed.

The higher levels of straylight in the NIR detector seem to be caused by light with a wavelength longer than the NIR can detect. As the exact spectrum of this out-of-band straylight is not known and cannot be measured with TROPOMI, a calibrated correction of this straylight contribution has not been implemented in the L1b processor. For in-flight situations it is estimated that the out-of-band straylight contribution will be somewhat smaller. In the suspected wavelength range the white light source from on-ground calibration has more output than the Earth radiance. How large the impact is on retrievals in the O₂-A-band, needs to be determined in-flight.

J. SWIR Straylight

SWIR straylight has been measured using the external tunable cw laser at 100 spectral positions and 100 spatial positions, yielding about 10,000 measurements in total. The dynamic range of a single measurement was increased to about 10⁸ by measuring at four different exposure times. The very short exposure time measures the light in the laser peak, while three (much) longer exposure times measure the stray light. Saturation of the laser-peak signals is allowed for the SWIR CMOS detector.

The results show that stray light is hardly dependent on spatial or spectral position of the peak, making a deconvolution-based correction relatively easy. Typically, the stray light in the SWIR channel is reduced by a factor of 10 - 20, in accordance with the requirement. Despite this, the Level-1b requirement of 0.25% for the

hole-in-the-cloud scenario is not met by a factor of three, mainly because the Level-0 stray light is too high by the same factor.

K. UVN Detector and Front End Electronics

During the on-ground calibration drifts of up to 1 % were observed in the electronic gain of the UVN detectors. Also offset showed drifts in addition to patterns ('residuals') over the detector.

To reduce the impact on the L01b output, the electronic offset correction is now a dynamic correction, the calibration key data is retrieved per measurement frame. This is only possible when the in-flight instrument settings are chosen such, that the read-out register and overscan rows are available.

The background correction is split into a dark current and a residual pattern correction.

The gain drifts were seen to be highest for high CCD output gain settings and low settings. It is recommended to avoid the high CCD gain setting in-flight for radiance and irradiance measurements. For low signals the accuracy of the correction is reduced. Apart from the mentioned exceptions the offset and gain accuracies are well within 0.6%. To reduce the impact of gain and offset drifts, regular calibration measurements need to be scheduled for the nominal operations phase E2.

The pixel response non-uniformity and the register non-linearity are both known within better than 0.6%. The register full well values of the UVN detectors and the overall instrument optical throughput pose restrictions on the maximum binning factors for the UVN detectors.

L. SWIR Detector and Front-End Electronics

The SWIR detector and its Front-End Electronics were characterized on unit level, and results have been reported previously [5].

V. CONCLUSION

All calibration key data for the TROPOMI L01b processor has been derived consistently with the use of the processor itself. The relative irradiance response calibration and the validation of the geolocation still need to be performed in-flight. The lower accuracy of the absolute radiance correction, the straylight correction and the instrument BSDF do have some impact on the absolute radiometric accuracy, however, the overall result is still of high quality and all key data is validated and self-consistent. The impact on L2 retrievals needs to be assessed with in-flight radiance measurements.

All GSE used resulted in a very efficient calibration campaign in which >85% of the time useful measurements were taken. Some redundancy was built in the campaign which was later used to cope with a few measurements that didn't work out as planned; some extra tests are now planned for the in-orbit commissioning. In conclusion, nearly all objectives have been met and the calibration campaign is marked as successful given the fixed duration of 125 days.

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