LuftBlick Report 2024001

About Pandora Lunar Measurements - phase 3

Final Report QA4EO WP2322

Version 1 - Apr 30, 2024

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1 Document Change Record

Issue	Date	Section	Observations
1	30 Apr 2024	All	First version

2 Summary and Conclusions

This is the report of the 3rd phase of the work package (WP) 2322 “Night-time aerosol and trace gasses columnar observations” of the ESA project QA4EO phase3[1] for the time period 1 May 2023 to 30 April 2024.

The primary goal of this WP was to probe techniques to extend the usability of column retrievals based on direct lunar measurements that suffer from scattered solar light especially during twilight conditions.

In a first approach we have adjusted the measurement sequence that includes off-moon measurements for the compensation of scattered solar light with the aim to enhance the coverage of measurements during twilight conditions. This could be achieved by skipping the measurements used to correct for the dark signal in the data correction (“dark measurements”). Furthermore, this routine was also extended to nocturnal conditions and it is shown that off-moon measurements during nighttime are sufficiently representative for dark measurements, too. This way the very same measurement routine is applied all the time between sunset and sunrise.

In a further step, the extension of direct moon measurements into daytime is used to prove that “passive” AMF-correction procedures (e.g. estimating AMF errors from O_2O_2 absorption) are unlikely to be carried out successfully. The remote atmospheric conditions of Izana where these investigations were carried out on the other hand allowed to prove that the direct sun-AMF is representative for the NO_2-columns retrieved from off-moon measurements while direct lunar AMF is of course representative for the diffuse corrected on-moon vertical columns. This further supports the assumptions that passive corrections techniques target different atmospheric light paths.

In a second approach, we could show that during sunrise and sunset conditions, where the direct solar beam is strongly contaminated by scattered light, the correction of the inelastically scattered part (from rotational Raman scattering) improves the retrievals at very high AMFs and smooths out the difference between edge of the day and nocturnal retrievals further.

Last but not least an additional source for the bias in NO_2-columns with respect to calibration shortcomings could be identified by different straylight patterns for non-perfect alignment when different diffusers are applied with respect to none in place.

[1] Quality Assurance for Earth Observation project [Statement of Work for LuftBlick], SERCO Contract QA4EO/SER/SUB/04, 2022.

3 Introduction

3.1 Ideas & Goals

This WP had essentially three major goals, which are briefly described, summarized, and concluded in the following:

Goal 1) Study different approaches for AMF corrections during solar twilight

"Active" correction techniques, like radiance measurements recorded next to the moon and close in time, have been prototyped already, further refinement is targeted. Feasibility studies towards "passive" correction techniques including modeling or aerosol proxies (like O_2O_2 columns as utilized in MAX-DOAS) were carried out.

Goal 2) Improving potential of Raman correction during twilight conditions

The goal is to improve the inelastic molecular scattering (Raman effect) in the retrieval algorithm, considering N_2 and O_2 (regular Raman correction, also referred to as "Ring" correction) for targeted species (here, NO_2) in direct sun and lunar measurements. To investigate the effects of inelastic molecular scattering in comparison to retrievals that incorporate no Ring correction or only regular Ring correction, a short sensitivity study is conducted.

Goal 3) Conduct tailored studies or experiments to isolate the source of calibration short comings

The source of the instrumental driven calibration discrepancy needs to be isolated. In particular, if the discrepancy is a result of a missing (hence not yet characterized) instrumental feature or an improper implementation of existing methods.

3.2 Official WP-description

PROJECT: QA4EO	PHASE: 3/3	WP: 2322
WP Title: Night-time aerosol and trace gasses columnar observations Company: LuftBlick WP Manager: Martin Tiefengraber		Sheet 1 of 1 Issue Ref: 1.0
Start Event: KO	Planned Date: 1/5/2023	Issue Date: 21/2/2023
End Event: FR	Planned Date 30/04/2024	WP Effort: 530 hours

30/04/2024

Inputs:

- Blick Software Suite Manual including the ATBD
- Scientific publications related to PGN, accuracy estimations and remote sensing measurements
- Final report of QA4EO WP2322 phase 1 and 2

Tasks:

- Refine existing "active" AMF correction technique, consisting of off-moon radiance measurements.
- Feasibility studies on "passive" AMF correction procedures, using modeling or aerosol proxies (e.g. O2O2 columns).
- Investigate the improving potential of applying Ring correction during solar twilight phases.
- Conduct tailored studies or experiments to isolate the source of the calibration shortcoming.

Outputs:

- Presentations at QA4EO workshops.
- Technical report "PGN Products Uncertainty Validation".

3.3 Acronyms and Abbreviations

AMF	Air mass factor
BSS	Blick Software Suite
DOAS	Differential optical absorption spectroscopy
FWHM	Full width half maximum
H_2O	Water vapor
LZA	Lunar zenith angle
MAX-DOAS	Multi axis differential optical absorption spectroscopy at multiple axes
MD	Direct moon measurement routine with diffuse correction
MLE	Modified Langley Extrapolation
MO	Direct moon measurement routine with open hole
MX	MD but diffuse correction replaces dark correction also for nocturnal conditions
MY	MX but also enabling daytime measurements of the moon
N_2	Molecular Nitrogen
NO_2	Nitrogen dioxide
NO_3	Nitrate radical
O_2	Molecular Oxygen
O_2O_2	Dimer of molecular oxygen
O_3	Ozone
PGN	Pandonia Global Network
QA4EO	Quality Assurance for Earth Observation
SC	Slant column
SZA	Solar zenith angle
VC	Vertical column
WP	Work package
wrms	Normalized rms of fitting residuals weighted with independent uncertainty

4 Refine existing AMF correction during twilight conditions

4.1 Improving the active diffuse correction to the lunar routines

Multiple scattering extends the effective light path (air mass factor, or AMF), leading to an underestimation of the direct (geometrical) AMF and consequently an overestimation of the retrieved vertical columns of NO_2. To address these inaccuracies, various correction methods have been developed in the BSS, particularly for direct NO_2 measurements during solar twilight. Active correction techniques, which involve radiance measurements taken near the target and close in time, have been prototyped but require further refinement.

During direct sun measurements, the increase in AMF due to multiple scattering is negligible (up to SZA ~85.°) because the diffuse component of sunlight is minor compared to the direct solar radiation (approximately 1/100,000 of the total light). Hence, no correction for this increase is necessary, as the apparent increase in NO_2 content due to the elongated light path is minimal.

However, the situation is markedly different during lunar measurements in twilight conditions, where the brightness of diffuse atmospheric sunlight is comparable to that of the moon. Here, the competing brightness from scattered sunlight necessitates corrections. An active correction strategy involves measuring the sky close to but without the moon and subtracting this measurement from the direct lunar irradiance, assuming that atmospheric conditions do not change significantly between these measurements neither spatially nor temporally.

To enhance these correction techniques, off-moon measurements taken at 8° difference in azimuth on both sides of the moon are also utilized for instrumental 'dark' correction under nocturnal light conditions with the Pandora 209s1 instrument located at Izana. These off-moon measurements, which represent the diffuse light in the surroundings, replace the previous dark measurement setup, thereby doubling the total number of measurements compared to the previous twilight routines. The frequency for actual nocturnal conditions is reduced by 2/3 (on-moon & “dark” vs on-moon & 2 off-moon measurements), which is a minor drawback. In this method, off-moon spectra are wavelength-corrected to create a synthetic on-target spectrum and temporally interpolated to match the on-target before subtraction. Spectral fitting is then performed only on the corrected on-target measurement. As shown in Figure LunarDiffuseCorrection, a comparison is made between a regular direct moon measurement (blue), corrected by dark measurements taken by using opaque filters, and a direct moon measurement (yellow) corrected by diffuse light. During twilight, the measured moonlight is a sum of direct moonlight and scattered (=diffuse) sunlight, creating an apparent increase in the Vertical Column (SC). By applying the diffuse correction, this increase in the SC can be diminished.

The Figure SketchDiffuseLight illustrates a scheme of the direct on-moon measurement, the off-moon measurements on both sides and the diffuse sunlight induced by the sun. It was observed that the intensity of the diffuse light differs between the off-moon left and right during sunrise and sunset, underscoring the importance of interpolating both measurements to estimate the contribution of diffuse light on the direct moonlight path.

All the previously mentioned routines cease as soon as the solar zenith angle is ≤ 90°. This restriction was removed in another testing routine, which allows measurements throughout the day, although it is limited by the moon phase, requiring at least a half moon. However, it has been observed that during periods before sunset and after sunrise, the diffuse light induced by the sunlight is much more intense than the lunar irradiance. Under such conditions, the effectiveness of the diffuse correction is diminished.

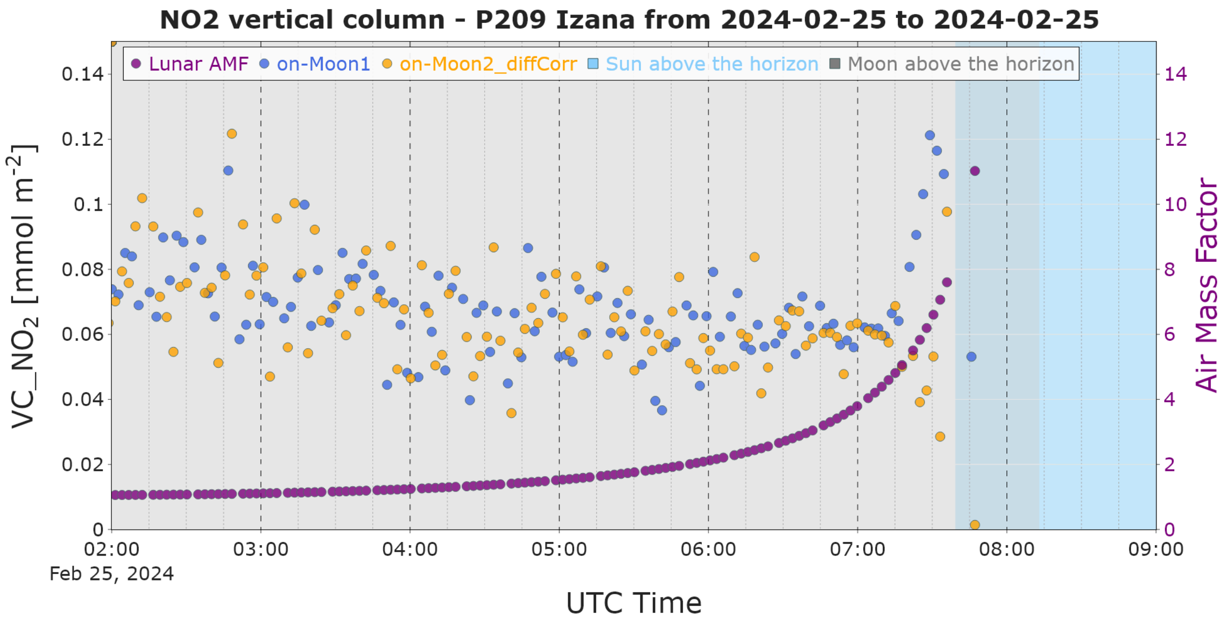
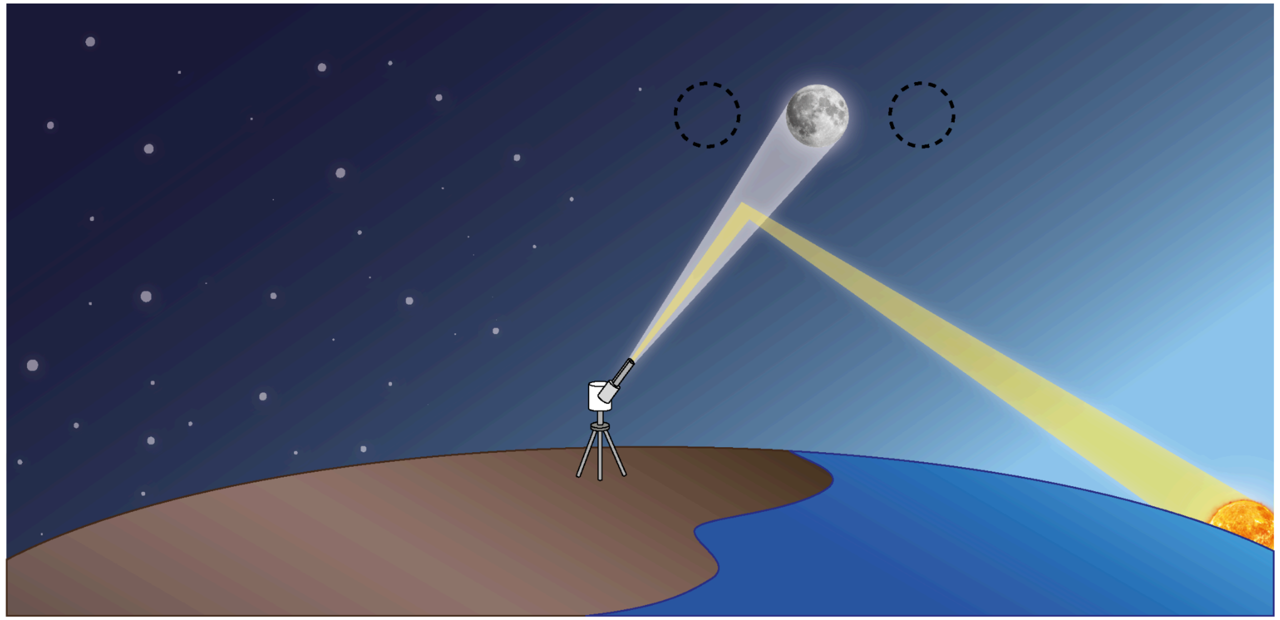


Figure LunarDiffuseCorrection: Impact of diffuse correction on direct lunar measurements. 'on-Moon1' represents the standard on-moon measurements, while 'on-Moon2_diffCorr' represents measurements corrected for diffuse light. The light blue and gray areas highlight the times of day when the Sun and Moon are above the horizon (zenith angle ≤ 90°), respectively. Notice that the on-Moon measurement without diffuse correction increases in the same proportion as Lunar AMF during the twilight period, whereas the diffuse corrected one follows the trend of the NO2 vertical column along the nighttime until the sunlight comes in.

4.2 Feasibility of passive AMF correction procedures to the lunar routines

The Figure SketchDiffuseLight further also illustrates the issues for identifying a possible passive correction procedure for the AMF (e.g. estimating AMF errors from O_2O_2 absorption). When collecting direct moon-data during twilight the sky scatters sunlight into the instrument with competitive irradiance with respect to moonlight. But these scattered sunlight, before being scattered by molecules and aerosols within the direct lunar path, already passed the atmosphere and interacted with all its species via scattering or absorption processes. So the information of the scattered sunlight reflects very different atmospheric conditions than the one reflected by the information of the moon light.



FigureSketchDiffuseLight: Diagram of the direct moon measurement, corrected for diffuse light induced by the sun during twilight. Note that both off-moon measurements are taken with respect to the azimuth angle.

So even if the alternative passive approach could involve estimating the increased light path of the diffuse light by measuring O_2 or O_2O_2 columns, this method does not appear applicable due to the unique atmospheric dynamics between the moon and the instrument.

In order to prove the assumption that the direct sun AMF is more applicable we also tried to retrieve NO2-vertical columns from the diffuse light. Especially during daylight conditions, the stable NO_2

situation (expected for the remote site of Izana) proves this approach applicable. And if the direct sun-AMF is applied the resulting vertical column is remarkably close to NO_2-vertical columns as retrieved from direct moon measurements as shown by blue and red dots for the times where moon and sun are both above horizon as shown by the overlap in lunar and solar retrievals for the days before full moon. The possibility to get meaningful values from diffuse light measurements already in twilight scenarios of course prove that MAX-DOAS measurements could be extended into twilight-scenarios.

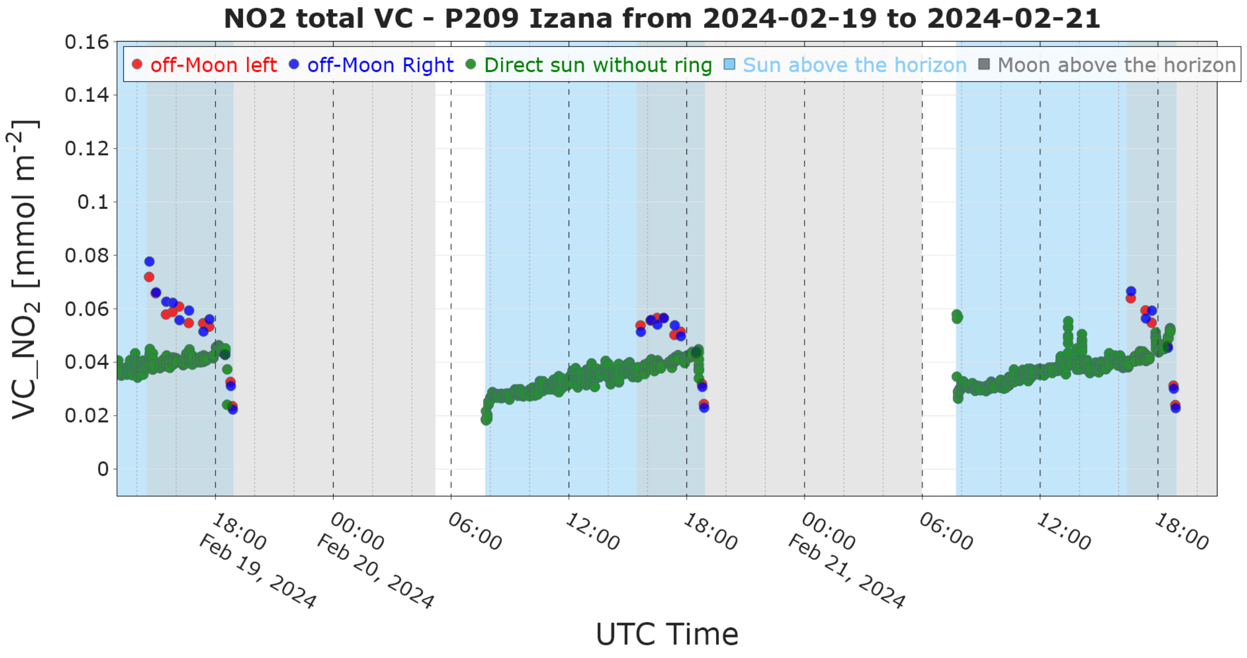


Figure DiffuseLightNO2Retrievals: Comparison of NO_2 vertical columns retrieved from direct sun measurements (green circles) and off-moon measurements ("diffuse light") (red and blue circles) measured 4, 3, and 2 days before the full moon. The gray background represents the moon above the horizon, and the light blue background indicates daytime.

4.3 Lunar routines compared with direct sun measurements

The following Figure DiffuseCorrectionAroundFullMoon2024 compares the NO_2 vertical columns (VC) from direct sun measurements without ring correction to lunar measurements with active diffuse correction applied during three specific times: four days before the full moon, on the full moon day, and four days after. The NO_2 VC during the full moon day shows less variability due to a major light intensity than the previous or after days, where the signal to noise ratio is higher.

Notably, there are gaps in both types of retrievals during sunrise and sunset on the days before and after the full moon, respectively. This is attributed to the moon's position below the horizon (Local Zenith Angle, LZA > 90°) during these periods.

The Figure Uncertainty&wrmsLunarDiffCorrected shows a comparison of the independent uncertainty (=measurement noise) and the weighted root mean square of the fitting residual (wrms) between the direct sun measurements, without any corrections, and the lunar measurements corrected for diffuse light on the full moon day. The lunar wrms values are observed to be at least one magnitude higher than those of the direct sun, which is also associated with the difference in light intensity between the two light sources.

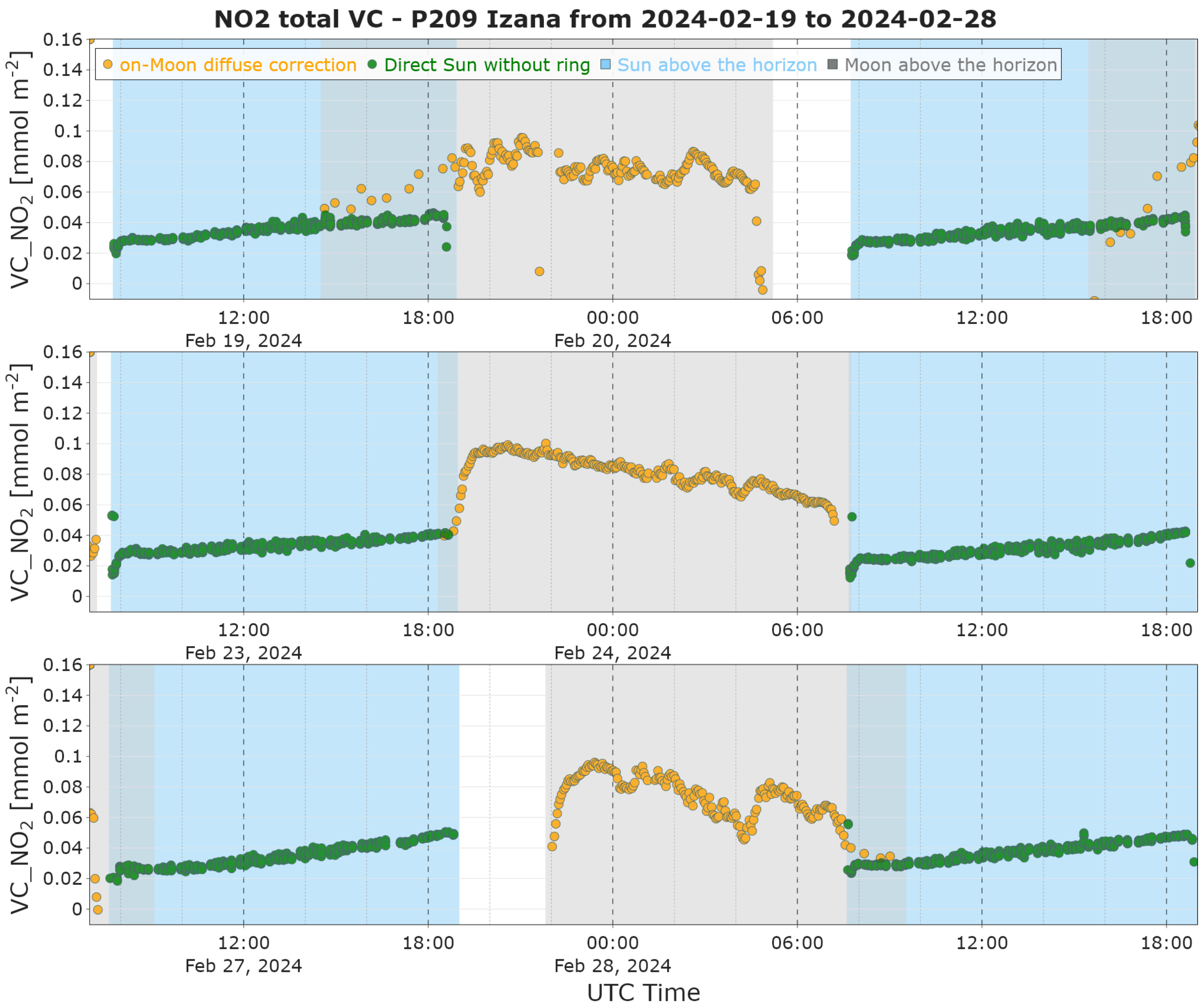


Figure DiffuseCorrectionAroundFullMoon2024: Comparison of NO_2 vertical columns measured four days before the full moon, on the full moon day, and four days after, with vertical columns obtained from direct sun measurements.

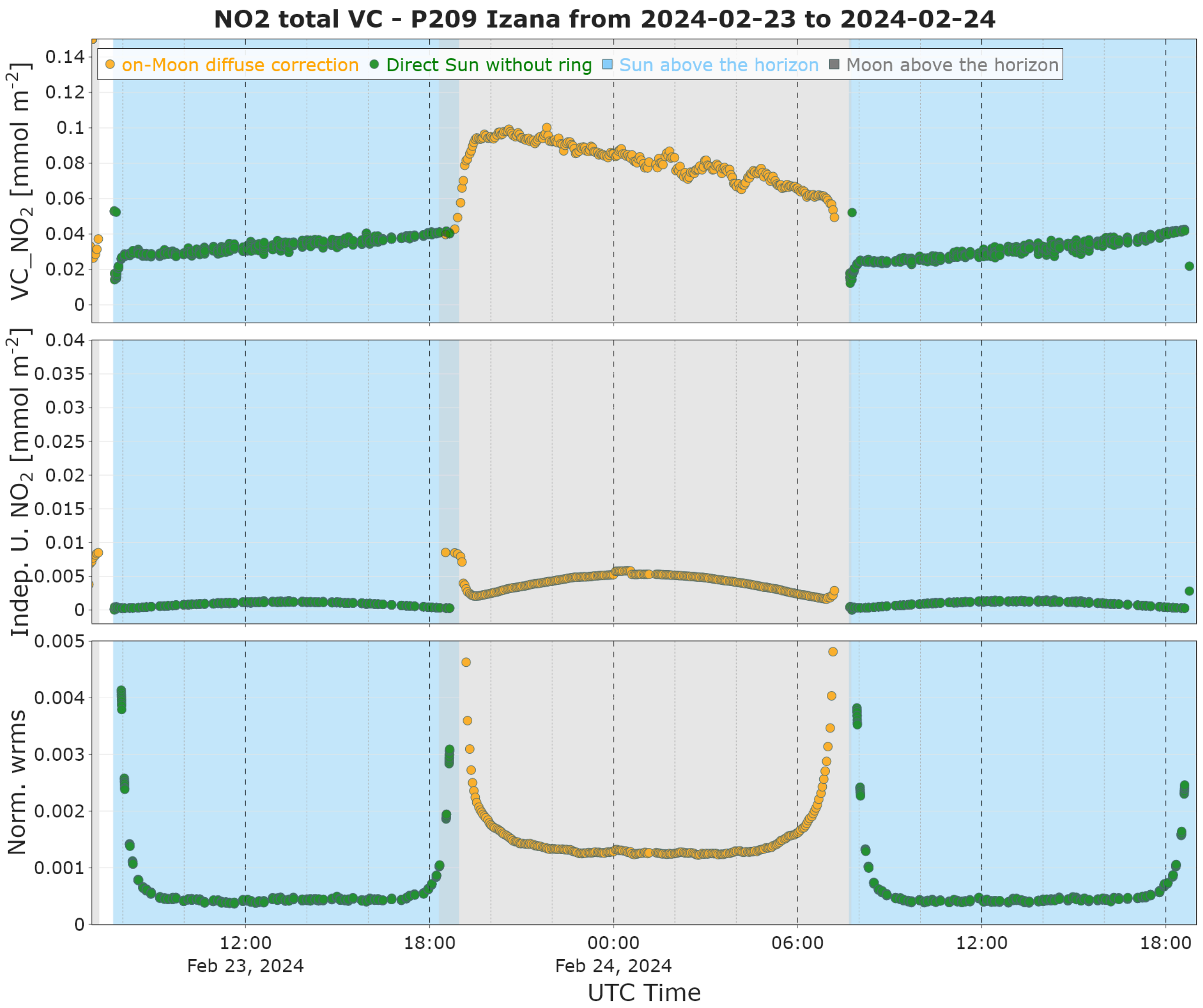


Figure Uncertainty&wrmsLunarDiffCorrected: Comparison of the independent uncertainty and wrms between direct sun measurements and lunar measurements corrected by diffuse light.

5 Effect of Raman correction (“Ring effect”)

5.1 Improving potential for direct sun measurements

Diurnal operational direct sun NO_2 measurements are a well-established data product of the PGN, but sunset and sunrise conditions still present some challenges. Enhanced scattered light contaminates the direct light path for direct sun measurements taken close to the horizon at large solar zenith angles. This leads to systematic biases in the retrieved slant columns if not properly accounted for. Until now, the inelastic part of the scattered sunlight was only considered for N_2 and O_2. In this study, we investigate the potential for improving the vertical NO_2 columns by explicitly considering the inelastic scattering for the target species, using data from the high-altitude background site at Izana (Pandora 209s1), where the (primarily stratospheric) NO_2 columns are well constrained. The results show that the Raman correction of this inelastic scattering component (referred to as “molecular ring” correction), notably enhances the previously underestimated vertical NO2 columns during sunset and sunrise conditions, aligning them more closely with lunar measurements (orange scatters). Concurrently, this correction substantially mitigates the bias observed in the slant columns. Figures MolecularRingDirectSun2022 and MolecularRingDirectSun2024 demonstrate that the molecular ring correction (indicated by red scatters) upwardly corrects the vertical NO_2 column immediately after sunrise and before sunset, respectively, in comparison with the regular ring correction and concurrently decreases the uncertainty and thus the wrms (as shown by red scatters). On 12th/13th September 2022 and on the 24th February 2024, the molecular ring correction not only reduces the decrease of the vertical NO_2 column after sunrise but also excessively increases it towards the lunar data (orange scatters), while still reducing the uncertainty. During daytime and, thus, for lower air slant columns, the effect of the molecular ring correction, compared to the regular ring correction, is almost negligible. Hence, the potential for improving vertical NO_2 columns through molecular ring correction is greatest at high solar zenith angles and smallest at noon, where scattering is generally almost irrelevant.

In conclusion, the attenuation of the molecular ring effect by the absorption of NO_2 only becomes significant at very high NO_2 slant columns/air mass factors which is exactly as expected.

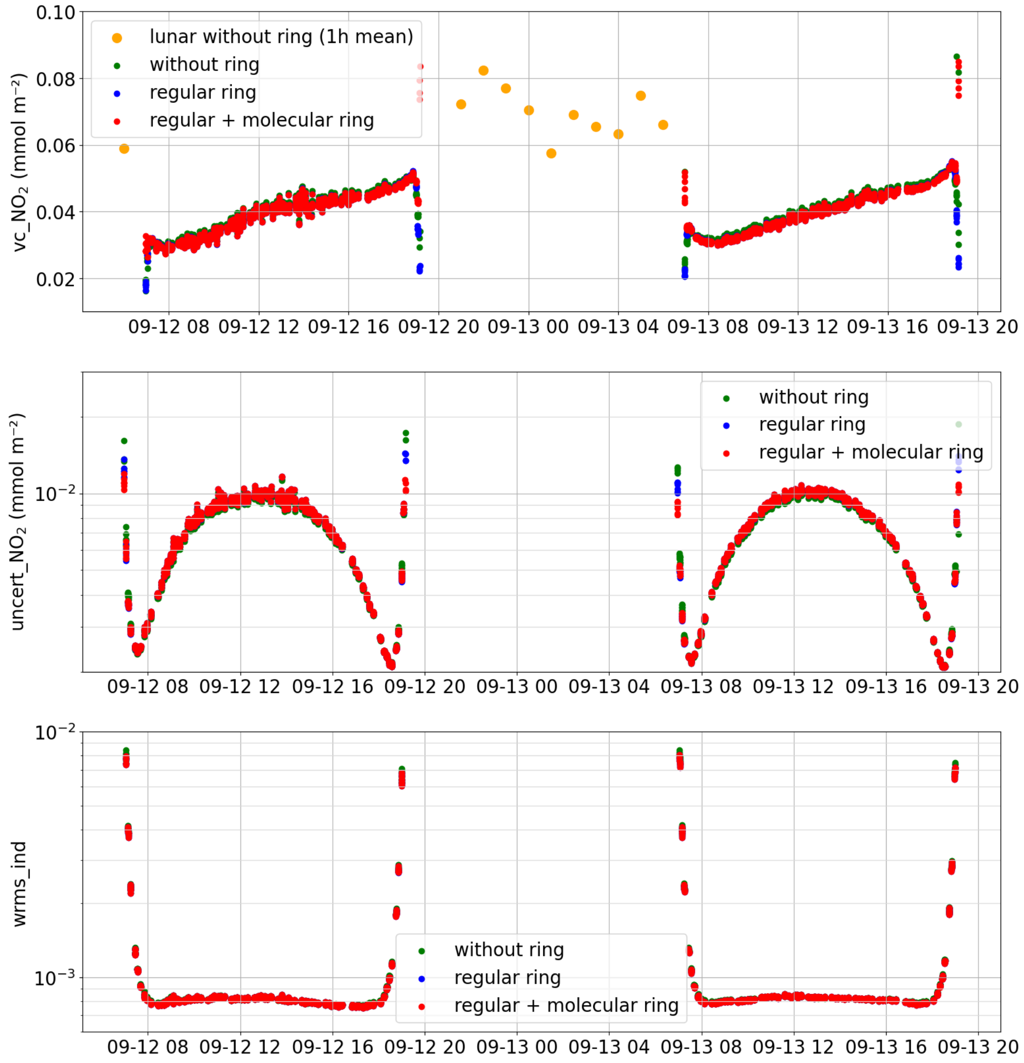


Figure MolecularRingDirectSun2022: Impact of molecular ring correction on direct sun and lunar NO_2 total columns.

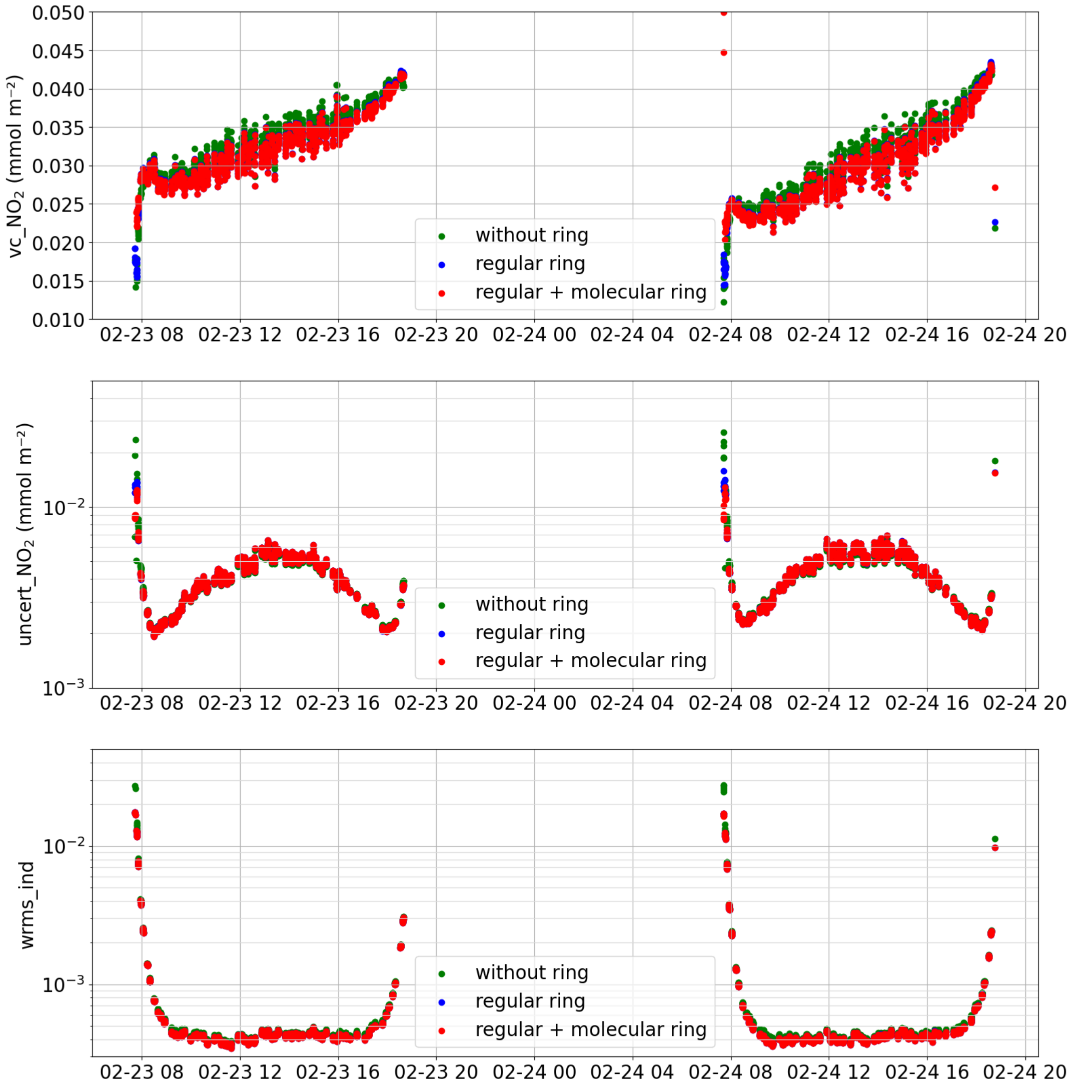


Figure MolecularRingDirectSun2024: Impact of molecular ring correction on direct sun NO_2 total columns.

5.2 Improving potential for direct lunar measurements

Lunar measurements bridge the twilight and nocturnal gap left by direct sun measurements, albeit with their own unique challenges due to the irradiance being 400,000 times lower. Particularly during twilight conditions, sunlight scattered by the atmosphere—which provides irradiance of a similar magnitude to that of the moon—significantly impacts the retrievals from direct lunar measurements. To correct for this, an active diffuse correction (off-moon correction) is applied, as explained above, theoretically resulting in conditions that represent only light originating from moon-reflected sunlight. In this way, the same conditions as for sunlight apply: irradiance of an order of magnitude 10^5 lower adds up to the lunar light. Ring corrections (effects of inelastic scattering) only show a non-negligible effect for high air mass factors. These very high lunar air mass factors significantly overlap with twilight conditions. Due to this, any impact of ring corrections applied to lunar light will remain significantly below the uncertainty resulting from diffuse correction. Therefore, no conclusive effect is expected on the final retrievals.

Figure ImpactMolecularRingCorrection illustrates this, by showing the effect of the regular ring (for N_2 and O_2) and molecular ring correction (for NO_2) across different lunar zenith angles, solar zenith angles during each lunar phase for the moon period from August 29 to September 20, 2022. It confirms that during solar zenith angles between 95-110°, the effect of the regular and molecular ring correction increases the vertical NO_2 column only slightly, by only 0.5-1.5 %, and in some cases, up to a maximum of 4 %. Overall, this analysis indicates that the potential for improving direct lunar measurements by applying molecular ring correction is very limited and almost does not affect the vertical NO_2 columns.

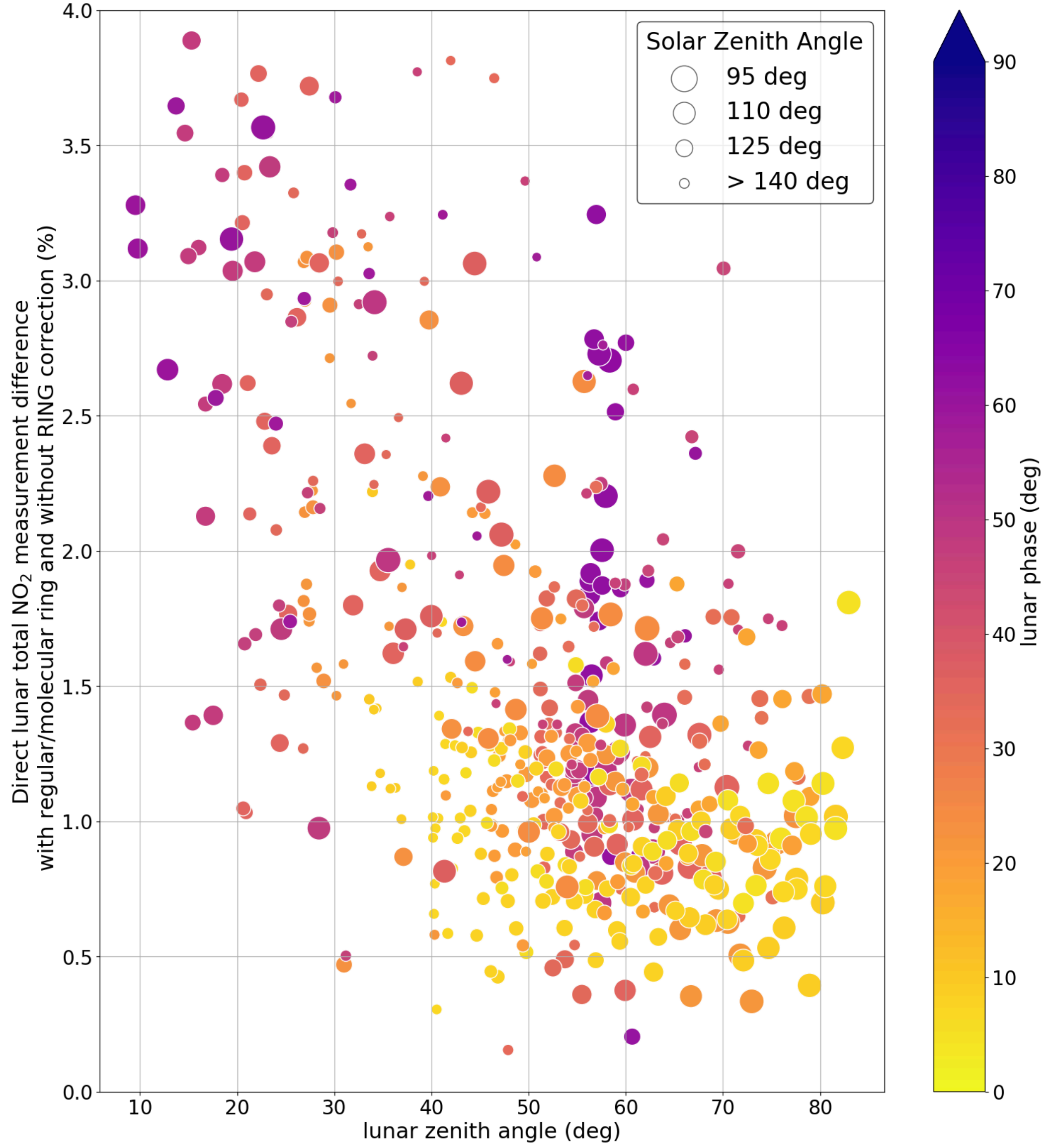


Figure ImpactMolecularRingCorrection: Impact of molecular ring correction on lunar NO_2 total column amounts.

6 Investigations on the reasons for the slant column biases

As pointed out in the report LuftBlick_QA4EO_PandoraLunarMeasurements_RP_2023007_v1 we investigate a bias in the retrieved nitrogen dioxide slant column depending on the reference the measurements were compared with.

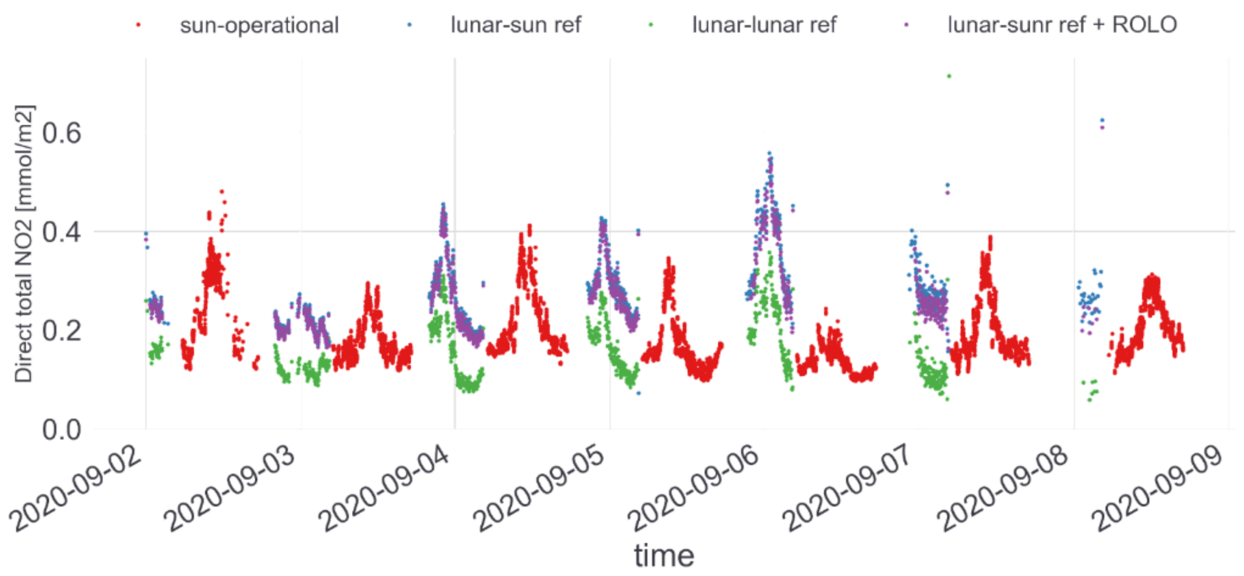


Figure LunarNO$_2$: Direct total NO$_2$ for Pandora 138 spectrometer 2 at Rome Sapienza for Lunar (green, blue, magenta) and direct sun retrievals (red).

This bias can be eliminated and is clearly related to the synthetic reference used for the retrieval. Either directly by changing the reference from being based on actually collected sun spectra to actually collected moon spectra or by evaluating the intrinsic NO2 slant column of this reference spectra, by MLE-statistics not based on retrievals from direct sun data but rather from direct moon data.

In conclusion the difference between the synthetic reference as retrieved from collecting direct moon data with respect to direct sun data manifests in an “artificial bias” (artificial meaning it cannot be a real bias) inherent to the instruments properties different for the 2 measurement setups.

Possible sources are:

1. Differences in sensitivity for different light intensities: The non-linearity extracted from standard bright analyses covering different countrates (UV-related pixels collect much less count rates) and counts (different integration times allow for the evaluation of count dependence) is too low for possible explanations.

2. Cross correlation effects between the thermal electron generation rate (dark signal) and nitrogen dioxide cross section. The dark signal being directly related to pixels rather than wavelengths is unlikely to have a significant effect on retrievals and on top of that the dark current is recorded with the same integration time shortly before and after the bright measurements. So an impact is unlikely.

3. Different optical elements used: Direct sunlight is measured with a diffuser in place. But due to low direct moon light intensity this diffuser is removed from the light path for nocturnal data acquisition: A non-perfect description of the instrumental characteristics with diffuser in place is therefore the most likely reason for the differences.

With respect to instruments designed for similar purposes Pandoras lack a pinhole spatial filter (lens-pinhole-lens-combination). This on the other hand enables the Pandora setup to even measure sky and lunar data and span measurements of irradiation differences of several thousand orders of magnitude. In our case spatial homogenisation is done by transmissive diffusers. The redistribution by the diffusive scattering effect yet is not as perfect with respect to a pinhole filter. Still it reduces light intensity inside the spectrometer by a factor of approximately 100. Therefore it is not in place for lunar and sky measurements, thereby eliminating any spatial homogenisation.

The imperfect characterization of the diffuser is therefore the most probable cause of the investigated bias. This assumption is further backed by the fact that we also investigate different biases for different diffusers in use. Apparently, the differences are not only related to the redistribution of the light but even depend on more detailed properties of these optical elements.

Within the last months we tried to identify the shortcomings of our description of the diffusers and could identify an impact on the stray light characteristics of the instrument. Yet this difference only becomes significant if the beam slightly deviates from exact alignment.

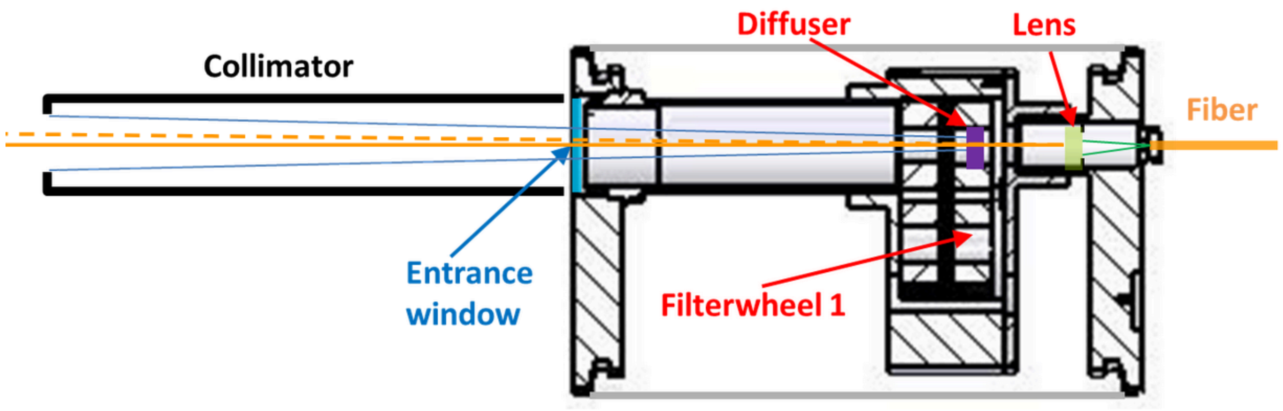


Figure Sensorhead: Sensor head with perfectly aligned beam (solid yellow line) and misaligned beam (dotted yellow line).

The following images are directly taken from the calibration software in use for characterizing instrumental stray light. The laser-wavelength of 450 nm was chosen for representing the different cases. This wavelength should be representative for NO2 retrieval which is extracted from fitting the wavelength range between 400 and 470 nm. The legend is found in the command line as indicated in the first image of the stray light pattern for a perfectly aligned ("on") instrument and different diffusers ("Diff 2" and "Diff 5") are compared to no diffuser in place ("open").

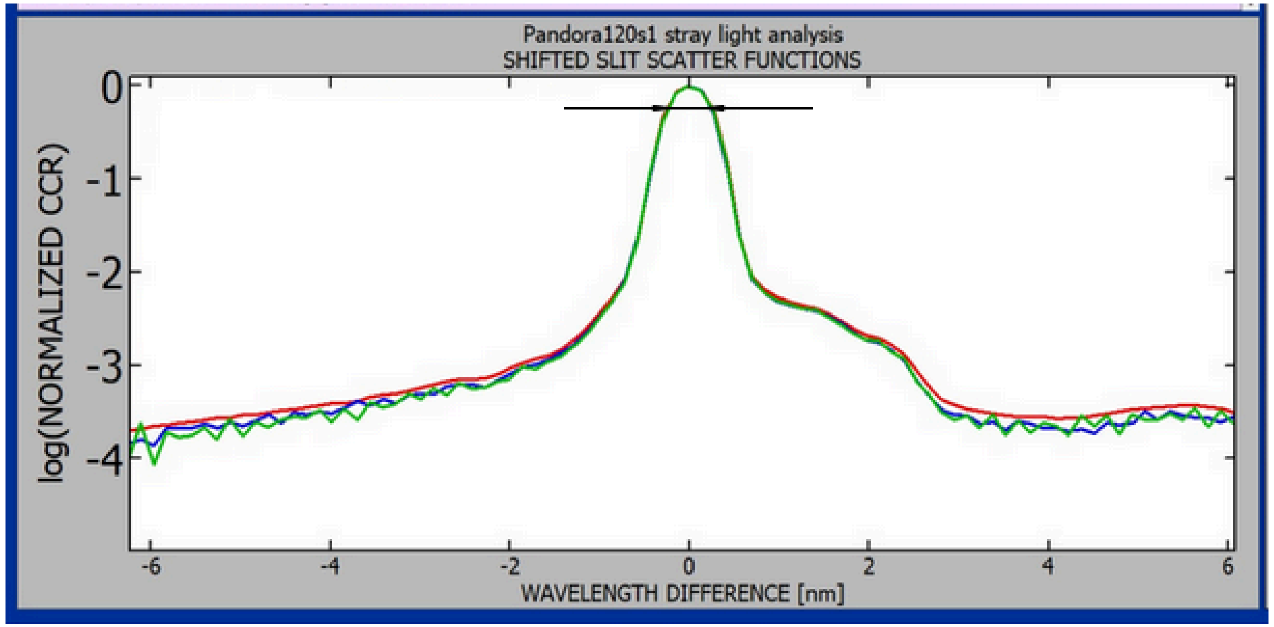


Figure WellAlignedStraylightPattern: Stray light pattern for a perfectly aligned instrument ("on") which refers to exactly the central and parallel incoming beam. Red arrow and rectangle indicate the legend as also found in the following images. The black arrow shows the full width at half maximum (FWHM) (log(0.5) = -0.3) of the laser beam representing the resolution of the spectrometer of appr. 0.6 nm.

The stray light pattern for all cases is very similar for a perfectly aligned instrument. This changes for a slight misalignment where the beam is approximately 0.05° of the optical axes. For open it slightly increases on the "right shoulder", for diffuser 5 it reduces on both sides and for diffuser 2 it reduces very pronouncedly. The different cases are shown separately in the following.

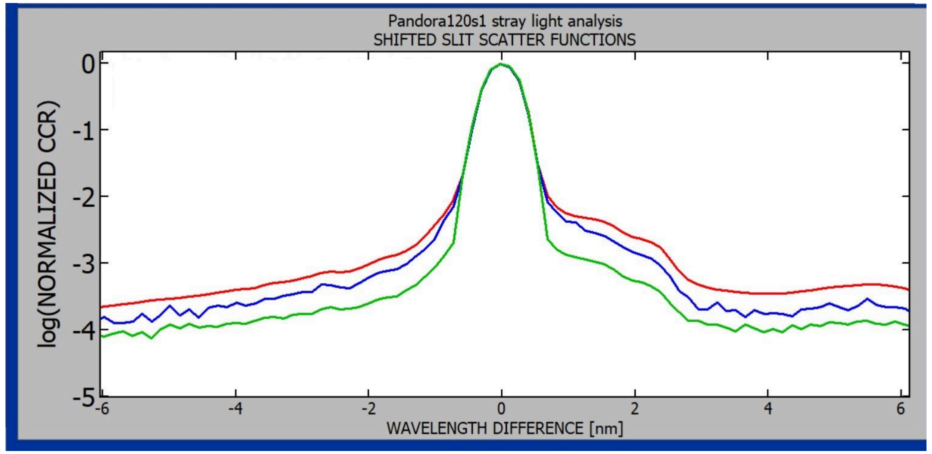


Figure MisalignedStraylightPattern:Stray light pattern for different diffusers in use for a slightly misaligned (off to the optical axes by 0.05°) instrument.

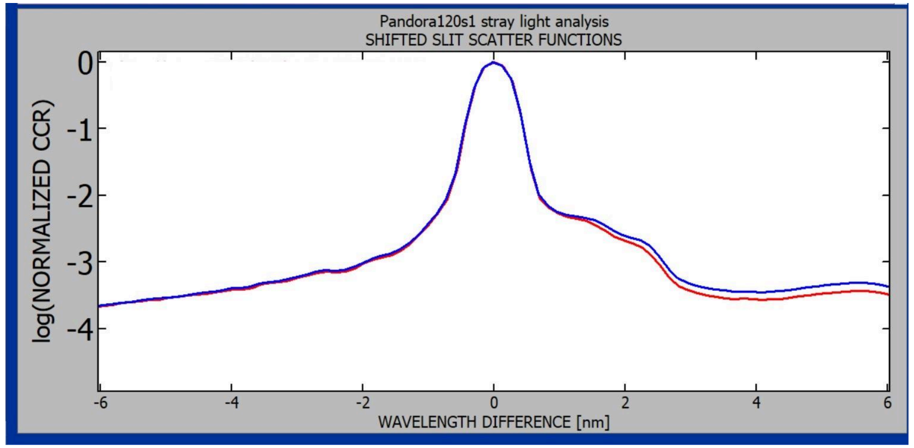


Figure AlignedVsMisalignedStraylightPattern_1: A slight misalignment of the instrument leads to a small increase of the right shoulder for no diffuser in place ("open").

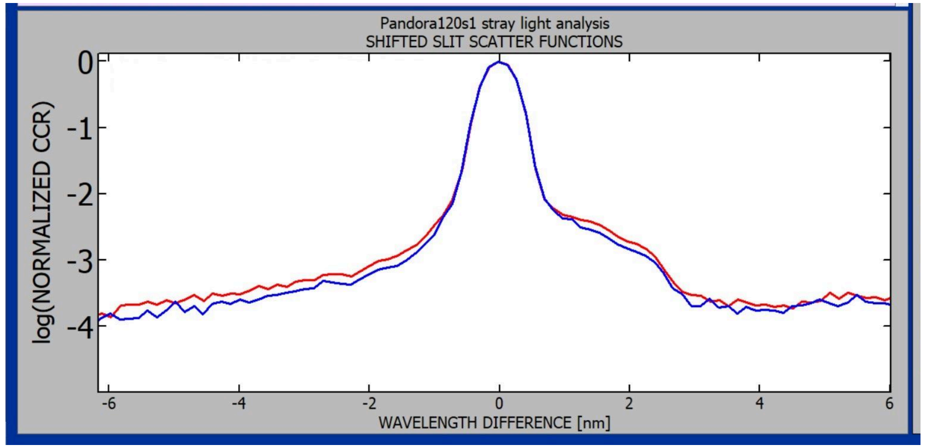


Figure AlignedVsMisalignedStraylightPattern_2:For diffuser 5 in use a slight misalignment ("off") of the instrument leads to a small decrease on both sides.

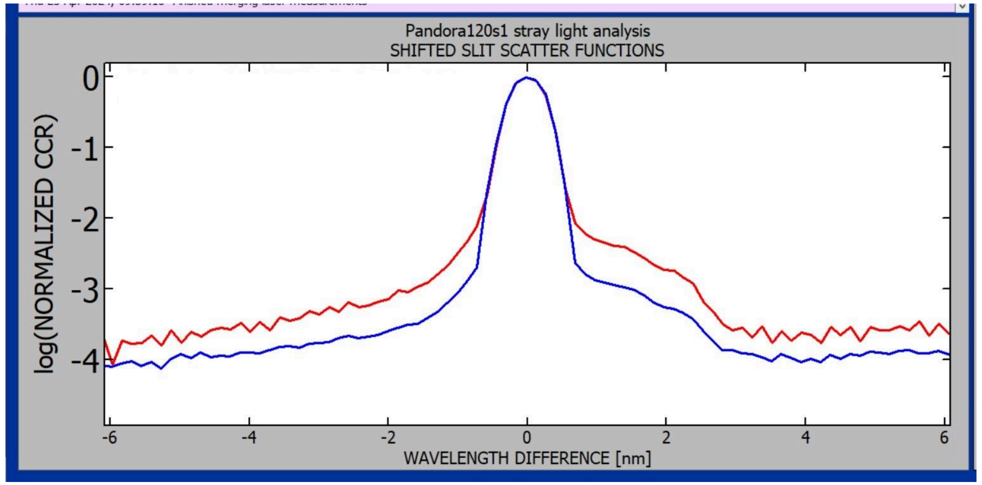


Figure AlignedVsMisalignedStraylightPattern_3: For diffuser 2 in use of a slight misalignment ("off") of the instrument the attenuation of the scattered light is more pronounced.

The stray light pattern represents an instrumental redistribution of light intensity. The laser light ideally would be reflected by delta function. In convolution with the non-infinitely small width of the entrance slit of the spectrometer the measured pattern still is mathematically well described by a symmetrically modified gaussian function. The full width at half maximum (FWHM) represents the resolution of the spectrometer with respect to wavelength. Due to the physical nature of laserlight there is no intensity expected for light of wavelength beyond approximately 3 times the resolution.

So stray light as the amount of light redistributed in difference to the ideal case is exactly addressing the parts where the differences are investigated. And there is a clear impact on this redistribution function.

Redistributing light in wavelength refers to a very similar effect as the so-called “ring effect” (see above). It equals an inelastic scattering and causes valley-filling/mountain-stripping if the off-core-part is increased and a valley-emptying/mountain-topping if decreased. Reduced stray light has the potential to convert into an increased slant column for the retrieval. So in the evaluated case the retrieval especially with diffuser 2 would result in a higher amount of NO_2 with respect to the open case. This exactly fits our investigations even if the instrument where the stray light characterization was done is not Pandora 138 where the retrieval was done. So one explanation would be that the reference spectra was collected with a not perfectly aligned instrument which is likely the case as the aimed maximum misalignment up to now is defined with 0.1° which is the double of the value where the “off-angle” stray light measurements were taken.

Yet this may not be the full story but it is a strong hint for where to focus in future investigations.

7 Future work

Based on the outcomes of this work package, some potential future working tasks can be concluded:

- Investigate the impact of **Raman correction** and **active diffuse correction** for other strong absorbers such as O_3 and H_2O during high AMF conditions.
- Conduct further tailored studies or experiments to **identify and possibly eliminate the source of the calibration shortcoming**.