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Atmospheric Measurement Techniques Discussions

Interactive comment on "Quantification and mitigation of the impact of scene inhomogeneity on Sentinel-4 UVN UV-VIS retrievals" *by* S. Noël et al.

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Reply to referee 2

We thank the referee for the helpful comments and will consider them in the revised version of the paper.

1 Answers to general comments:

The article addresses an important question in the development of retrieval algorithms for hyperspectral UVN instruments for atmospheric chemistry. With changes, the article should certainly be published. There are some areas in the text that require clarification before publication. Some of the figures will need to be updated with bigger lettering and some perhaps with a more convenient color scale. I miss a discussion of the applicability of this study to other spectral regions, in particular the NIR channel. The oxygen A-band itself may cause an inhomogeneous illumination of the spectral slit, i.e. the reflectance ratio may itself (strongly) depend on the wavelength. For the trace gases considered in the present form of the article this is not an issue, but for the oxygen A-band this most likely isn't the case. Without showing actual results the authors mention that the method is applicable. Further evidence of this is appreciated.

Text and figures will be updated as described below.

The present study concentrates on the UV-Vis spectral region, the results are not necessarily applicable to the NIR where the situation is in fact much more difficult. We only mention the NIR spectral region in the description of the spectral calibration algorithm. This algorithm also works in the NIR (in the sense that the spectral calibration works), but this does not mean that this is sufficient to mitigate the effects of inhomogeneity in the NIR. Since the performance of the spectral calibration algorithm in the NIR is indeed not shown in the paper and also not relevant for the present study we will remove all references to the NIR in the manuscript. We will furthermore mention more often in the text that our investigations are limited to the UVN UV-Vis band.

2 Answers to specific comments:

2.1 Scene description

The scene description given on page 2047, lines 16 – 19 is not consistent with the latitude where the spacial resolution requirement mentioned in footnote 1 is given. The latter can be found on page 2048. The time given in this scene description is not consistent with the time of overpass of the reference scene as observed by MODIS, as shown in figure 1 either. This is probably inconsequential, but using a consistent set of parameters is highly recommended.

The latitude specified in the footnote on page 2048 refers to the requirement on the UVN spatial sampling distance (SSD) only (which is 8 km at 45 deg latitude). As stated in the footnote, we assume the SSD to be constant in the context of this study, so it is assumed to be also applicable to the simulated scene.

The geometrical/time settings used in the radiative transfer calculations as described on p. 2047 are indeed not consistent with the selected MODIS scene, but this is not necessary as we want to assess the impact of scene inhomogeneity only. The inhomogeneous ISRFs calculated from MODIS data do not depend on the absolute radiances, only on the relative variation over the observed scene. The error mapping procedure is also quite independent from the selected radiance scenario, as long as 'inhomogeneous' and 'true' radiances are based on the same scenario (which is the case here).

2.2 Reflectance ratio

On page 2048, in equation 1 the reflectance ratio is defined. This definition is not symmetric, and I wonder if this is indeed the most practical definition. Have the authors

considered something similar to

$$RS = 2\frac{L_{left} - L_{right}}{L_{left} + L_{right}} \tag{1}$$

as a "reflectance symmetry". It has the property that it is symmetric with a sign change when L_{left} and L_{right} are interchanged, and ranges from -1 to 1.

We agree that the "reflectance symmetry" as proposed by the referee would also be suitable to classify inhomogeneous scenes and maybe really has some advantages compared to the definition of the reflectance ratio used in the present study. However, we use the reflectance ratio only in a qualitative way to classify different ISRFs / scenes. We do not claim that our definition of RR is the best choice, but looking at the results of this study this seems to work well. Anyway, both definitions (RS and RR) may be easily transformed into each other. Furthermore, the main conclusions of the study, i.e. the reduction of errors due to spectral calibration, are not affected by the definition of the reflectance ratio. Therefore we see no need to use a different definition in the context of this study.

2.3 Cloud fractions

The MODIS cloud fractions are determined from thermal infrared observations. However, the threshold values for the visible channel are determined such that the averages are the same. This requires a more thorough explanation. Thin cirrus may be given too much weight in this method, leading to a higher level of cloudiness than is actually visible.

It is agreed that the determination of cloud fractions (CFs) for the visible channel based on a combination of (visible) reflectances and CFs from thermal infrared data may result in too high values due to the larger influence of cirrus clouds in the thermal infrared. However, the derived CFs are not used in the error mapping procedure, they are only used to define a sub-group of results (in this case those for CFs $< 20\%$) which is considered to be most appropriate to derive tropospheric information. This threshold of 20% is based on experience from other instruments/retrievals and has to be verified as soon as real UVN data are available. Therefore the absolute accuracy of the derived CFs is considered to be not critical for the present study.

We will mention this in the paper.

2.4 Reflectance

The authors use a definition of reflectance on page 2050 in equation 2 that is a direct ratio of radiance and irradiance. They then explain in a footnote that there are other definitions. This is confusing. Please call the direct ratio "Sun normalised radiance", or use a definition of the reflectance which scales to the range [0, . . . , 1], i.e. $L = \pi I/(\mu_0 R)$. *It is agreed that this is not relevant to the study, but this type of confusion should be avoided.*

To clarify this we will modify this section as follows:

The sun normalised radiance L is defined as the ratio of radiance to irradiance:

$$L := \frac{R}{I} \tag{2}$$

In the context of this study L is equivalent to a reflectance which is usually defined in a similar way but including additional geometrical factors, like the cosine of the solar zenith angle. This difference is however not relevant here, because these factors do not have a spectral dependence.

2.5 Retrieval and error mapping

The description of the retrieval method in section 2.5 is very minimalistic, and should be expanded. While optimal extimation as written down by Rodgers is a well known technique, there are many implementation details that affect the output. A discussion of the retriaval bias and retrieval precision is needed. Also the description of the role of the a-priori information should be expanded. Op page 2052, lines 3 – 8, the authors mention that the error analysis is incomplete, and separates out the error on a single parameter. They imply that this error is the error due to inhomogeneous slit illumination. In my view further clarification of this paragraph is needed, as it plays a central role in describing what is shown in the article.

We will re-write section 2.5 to explain this in more detail. Especially we will avoid the term ‘retrieval’ in the text, because we did not perform a full retrieval but an error mapping based on the optimal estimation method, using the formulas given in the Appendix.

The updated section will read as follows:

The information content and error analysis approach is based on the Optimal Estimation retrieval scheme and performance assessment (see e.g. Rodgers, 2000). Optimal estimation combines the information from the measurement with a-priori information of the parameter to be retrieved.

Instead of a full retrieval, an error mapping is performed. We assume a moderately linear problem (i.e. neglecting non-linearities) to determine the errors. The formulas for this approach are given in Appendix C. As a-priori state, the simulated state of the atmosphere is used. The linearisation of the forward model is performed around this a-priori state. The forward and instrument model is used to simulate the a-priori radiance. Here, the instrument model is assumed to be insensitive to the inhomogeneity of the scene, i.e. we simulate a homogenous illumination of the slit and use the homogeneous ISRF to calculate the spectra from the mean radiance of the scene. The inhomogeneous ISRFs are then used in the instrument model to determine how the measurement of the radiance is disturbed by the inhomogeneous illumination of the slit. The difference between the erroneous radiance and the true radiance is then mapped to a difference between the true state (which is also the a-priori state) and the state a retrieval would determine from the erroneous radiance. This difference estimates the size of the systematic error we get from the inhomogenous illumination of the slit and therefore from the inhomogeneity of the scene.

The systematic error would appear in a retrieval as a bias. The precision of an optimal estimation retrieval is determined by the covariance of the radiance measurement (i.e. the noise) and constrained by the a-priori covariance. In this manuscript emphasis is placed on the minimisation of the systematic errors.

In the error mapping model, four trace gases are considered: O_3 (fitting window 305–330 nm), NO_2 (405–500 nm), SO_2 (308–325 nm), and HCHO (337–360 nm). For all quantities, the profiles of the scenario as specified in Tables 1 and 2 are used as a-priori with an associated error of 50 %.

Note, that the error mapping is always performed for only one of the trace gases. It is assumed in the analysis, that the atmospheric state is perfectly known for all parameters except the retrieved one. Potential impacts of scene inhomogeneity on other retrieval parameters are not considered in the context of the present study. The only instrumental effect taken into account is the inhomogeneous illumination of the slit. A small error for a geophysical parameter due to a single instrumental error does not necessarily mean that this parameter can be retrieved with the estimated error. A full error budget needs to be built up for all instrumental limitations, also including errors introduced by the imperfect knowledge of e.g. cloudiness, surface albedo or aerosol loading. Since such an error budget would depend on the actual retrieval method it is beyond the scope of the current study.

2.6 Results

The effect of the wavelength calibration is discussed in section 3. However, the size of the wavelength shift itself is not given.

Spectral shifts are different for each scene and also depend slightly on wavelength. The mean spectral shift for all scenes is close to zero, i.e. positive and negative shifts cancel on average. The mean absolute shift is about 0.005 nm, the maximum absolute shift is about 0.04 nm.

We will mention this in the text.

2.7 Conclusions

More quantitative conclusions may be drawn. The three separate conclusions on page 2054, lines 7 – 12 are rather qualitative, while numbers are avaliable elsewhere in the article. The last part of the conclusions were not discussed earlier in the article. While plausible, they should appear earlier on. The conclusion as given here seems in contradiction with the good results obtained in the error analysis and error reduction. Further details are needed why additional attention to the effect of inhomogeneous illumination of the spectral slit in the on-ground calibration phase is needed.

We quantify the tropospheric column errors (about 5% mean error, 50% maximum error) and also the error reduction due to spectral calibration (up to a factor of about 10 for the mean error, resulting in mean errors well below 1%). Especially, we will also mention in both the conclusions and the abstract the standard deviation of the errors (up to 8% before, 1.5% or less after wavelength calibration), as this is a measure for the additional uncertainty of a derived product introduced by the inhomogeneous illumination conditions. The quality of the reflectance ratio as a measure to characterise inhomogeneous illumination can not really be quantified, as there is no reference measure for inhomogeneity. Therefore we mention the correlation between the derived errors and the reflectance ratio (correlation coefficient ± 0.7) in this context.

There is no contraction between the recommendations given in the last part of the conclusions and the previous results. In the context of the present study the inhomogeneous ISRFs are only used to derive representative radiances from inhomogeneous scenes. In the spectral calibration and the error mapping only the homogeneous ISRFs are used. For the simulations described here this is sufficient to significantly reduce the errors of the tropospheric columns. However, the characteristics of the real instrument, which will be determined during on-ground calibration, will probably differ from the ones assumed in this study. Another aspect is that the actual retrieval method used to determine the tropospheric columns (in contrast to the simple error mapping approach used in the present study) might introduce additional uncertainties, e.g. due to limited knowledge of surface albedo or cloudiness and the inhomogeneity of these quantities over the observed scene. Therefore it is recommended to repeat this analysis once the real instrument properties are known. If in this case the spectral calibration will turn out to be less efficient, additional mitigation strategies need to be considered. One of these strategies could be to estimate inhomogeneous ISRFs for a specific scene based on sub-pixel information obtained in-flight during the scan. These estimated ISRFs could then be used in the retrieval instead of the homogeneous ISRFs.

We will add a paragraph in section 3 explaining these issues a bit more and also reformulate the conclusions accordingly.

2.8 Inhomogeneous ISRFs

I found appendix A hard to read, but after careful reading I believe this is correct. However, I miss a discussion on the limitations of the modeling of the inhomogeneous illumination. Does an inhomogeneous illumination of the spectral slit lead to an inhomogeneous illumination of the dispersive element? If so, what is the impact of that on the width of the slit function?

There is no image of the slit at the dispersive element, therefore the impact of inhomogeneous illumination of the slit should be very low.

One limitation of the approach is however, that we concentrate in this study on the impact and mitigation of inhomogeneous illumination in across-slit (spectral) direction. For the UVN UV-VIS band this is sufficient, because there is from design almost no spectral smile (i.e. no variation of spectral calibration in spatial direction). For other instruments or spectral bands this might not be the case, such that also inhomogeneities in the along-slit (spatial) direction may have an impact. In the construction of new instruments also hardware solutions to avoid inhomogeneous illumination of the slit using e.g. spatial scrambler units as proposed by Gerilowski et al. (2011) should be considered.

We will mention this in the introduction and in the conclusions.

2.9 Spectral calibration

The authors introduce equation B5 on page 2060 for the spectral calibration of radiance spectra. They state that this can be used for oxygen in the NIR channel, using equation B6. They state that this is a DOAS-type method. Applying a DOAS like technique to the oxygen A-band is likely to end in tears. The authors should either explain in detail how this can work for the oxygen A-band, or remove references to the NIR channel.

The spectral calibration algorithm as described in Annex B has in fact shown to work also for the NIR, although things are indeed a bit more complicated in this spectral region. In the context of this study the performance in the NIR is however not relevant, therefore we will remove the references to the NIR channel.

3 Answers to technical corrections:

- *Page 2044, line 12. Be specific. "It could be concluded. . . " is vague. Suggest to use "We conclude".*

  Will be changed.

- *Page 2044, line 16: "by factors up to $>$ 10". Suggestion to write "by factors up to 12", as this is the actual maximum in table 3, or use "by factors up to about 10".*

  Will be changed.

3.1 Comments on the figures

Fig 2 *A cloud frction is given without further details in the caption. Describe its source here. The colorscales are not adequate. Many pixels fall into the same color-bin, this could be addressed by selecting an appropriate range. Panel d has a clear central value (either 1 or 0 if my suggestion for RS is followed). The colorscale should reflect this.*

The cloud fractions have been calculated as described in section 2.2. This will be mentioned in the caption.

The fact that many pixels fall into the same colour bin is due to the selection of a quite cloud-free scene. We will adapt the ranges to increase the contrast. For the reflectance ratio we will adapt the colour scale such that it is centred around 1 (i.e. using a blue-white-red scale where white is associated to RR=1).

Fig 3 *The lettering is too small.*

We will increase the font size.

Fig 5 *The lettering is too small. The color combination is especially hard on (most) colorblind readers.*

We will increase the font size and replace the green crosses by blue ones.

Fig 6 *The lettering is too small. Mention the abbreviation in the caption (CF = cloud fraction).*

CF will be mentioned in the caption and we will increase the font size. Note that this is intended to be a full page figure in AMT (rotated by 90 deg), which will additionally increase the lettering.

Fig 7 *Mention the abbreviation in the caption (SC = spectral calibration).*

SC will be mentioned in the caption.

Interactive comment on Atmos. Meas. Tech. Discuss., 5, 2043, 2012.