Authors' response to referee #1, Isabelle De Smedt, comments on "Smithsonian Astrophysical Observatory Ozone Mapping and Profiler Suite (SAO OMPS) formaldehyde retrieval"

We will like to start by thanking the referee for the thoughtful and productive comments. This comments are helping us to improve our paper. In the text that follows each one of the referee comments is going to be copied in black with our answers in blue. How we propose to change the manuscript is shown in purple.

Too many qualitative affirmations are given in the abstract and in the rest of the paper. The impact of the OMPS and OMI different spatial and spectral resolutions on the detection limits should be better quantified and discussed.

Our answers to particular comments address the issues about detection limit and its relationship with spectral and spatial resolution.

The description of the method to select an optimal fitting window is difficult to understand, see the specific comments. While the selected fitting window is certainly appropriated for H2CO retrievals, the explanations are not convincing. This part needs to be improved.

Our answer is detailed in the specific comments section.

The discussion of the AMF error contains some shortcomings. For one particular parameter, the given error estimates will depend on the other parameter values, and on the profile shape. For example, an error on the cloud pressure will have a different impact on the AMF depending on the profile shape. This is not discussed at all.

Again we have addressed this concern in the specific comments.

Sections 4 should be extended. Comparison with NASA OMPS formaldehyde product (Li et al., 2015) is missing, since a direct comparison of two different algorithms applied on the same instrument would bring interesting information on the products. It is not clear why two OMI products are used in the comparison. Furthermore, the use of the BIRA OMI product v14 needs to be verified. Averaged columns over some regions do not match the gridded files distributed on the TEMIS website, in particular over the Pacific Ocean and Southern Africa.

The main reason we used BIRA OMI and SAO OMI is because these two products are freely available. We believe it is interesting to start comparing products from the same instrument produced by different groups. The recent paper by Zhu et al. (2016), which you are a co-author in, is a clear example of the value of this comparisons. We asked Can Li for data. Unfortunately he has not processed data for the full period of time we are using. He is also planning on using the new L1B recently available for OMPS to process a new version of his HCHO. We are keeping a close eye on each other product to be able to carry on a comparison study between OMPS retrievals once the new versions are ready (We are also planning on reprocessing using new L1B data).

Specific comments:

Abstract, p9210, line 17: Please explain how the detection limit (7.5e15 molecules cm⁻²) is derived from RMS (5e⁻⁰⁴)

We have estimated the detection limit by calculating the relation between the RMS and the H_2CO cross sections. The idea is that any SCD that will make true the following expression will be detectable:

$$SCD \times \sigma_{max} > RMS$$

 σ_{max} is the maximum H₂CO cross section in the fitting window. If we consider laboratory cross sections with an approximate spectral resolution of 0.005 nm this calculation results in a detection limit of ~3e15 molecules cm⁻². After convolving H₂CO cross sections with OMPS slit function (spectral resolution ~1nm), we get a detection limit of ~7.5e15 molecules cm⁻². This text is going to be added in page 9216 line 11.

"... molecules cm⁻². This estimation assumes that any SCD with an associated optical depth higher than the RMS is above the detection limit. As the background ..."

Intro, p9211, line 16: Please add reference to Stavrakou et al., 2014...

Added.

Intro, p9211, line 27: Please add reference to De smedt et al., 2015...

Added.

Section 2.2.1, p9213, line 26: the GOME, SCIAMACHY, GOME-2 and OMI H2CO retrievals from BIRA product are all performed in the 328.5-346 nm window. Please correct.

We have now corrected the text. Now it reads:

"..., different to that used in several consistent GOME, GOME-2, SCIAMACHY, and OMI retrievals, 328.5 to 346 nm, that do not include the H_2CO absorption band located around 353 nm."

Section 2.2.1, p9214, Figure 1: What is shown on the figure? The correlations between the cross-sections or between the fitted SCDs along one orbit? From the second part of the legend, I would say that these are correlations between SCDs. Please clarify the legend and the text. Please specify which orbit has been used, and the step of the fitting window wavelength increment.

Figure 1 shows the correlations between the fitted SCDs along the orbit. The main text is modified as follows:

"Figure 1 shows the correlation among H_2CO SCDs and the rest of the fitted SCDs for orbit 3538, an over pass of the Americas the third of July 2012".

And the figure caption:

"Correlations among H_2CO SCDs and other gas SCDs included in the fitting for different windows. The parameter space of the fitting window extremes was explored in 0.1 nm increments. The value of the x-axis indicates the beginning of the fitting window and the y-axis the end of it. The correlation values plotted here are the mean values for all the pixels in orbit 3538. Only pixels..."

Section 2.2.1, p9214, line 5: In the middle and right panel of Figure 1, the increased correlation between HCHO and O3 below 328 nm is not apparent. Correlation between absorption cross-sections is not the reason why wavelengths shorter than 328nm should be avoided, but rather the increase of ozone absorption (SCDs)

This is exactly what the text says "... two different considerations prevent the use of them. The first one is from the increasing strength of O_3 cross-sections below 328 nm, apparent by increasing values of the correlation between H₂CO and O_3 in the middle and right top panels of Fig. 1." We are going to remove the second part of the sentence where we make allusion to an apparent increase of the H₂CO/O₃ correlations which is not obvious at all. Thanks a lot for pointing this out.

Section 2.2.1, p9214, line 7: There seems to be a confusion between the O2-O2 and molecular Ring, at least in the text, and maybe also in the Figure. The description of the correlations do not match the subplots (on Figure 1, the correlation with Ring does not increase at shorter wavelengths). Beside, why is the term "molecular Ring" used? The first order of the Ring effect is not on molecular absorption but on Fraunhofer lines.

Again we agree that the whole explanation of the fitting window is too vague in the original text. We are re-writing this second part as follows.

"... prevent the use of them. The first band of low H₂CO-BrO correlations, below 326.5 nm, is discarded due to the increasing strength of O₃ cross-sections below 328 nm. The second band is discarded by the increasing correlation between the cross-section used to account for the Ring effect above 328 nm for fitting windows ending above 356 nm and the increase in correlations between O₃ and H₂CO above 330.7 nm. Another factor we have considered to select the fitting interval is to minimize fitting uncertainties (by increasing the number of spectral points considered). Extending the fitting window above 345 nm allows us to include the H₂CO absorption band centered at 353 nm. Including this band also implies including the wing of the O₂-O₂ band centered at 360 nm. To minimize the correlation between H₂CO and O₂O₂ we decided to start the fitting window at 327.7 nm and to include the H₂CO absorption band at 353 nm we chose as finishing wavelength 356 nm."

We use the term molecular Ring to refer to the Ring effect. We use this term to differentiate it from the contributions to the Ring effect due to vibrations of liquid water. In this region of the spectra we do not use this contributions from liquid water. For that reason we are going to remove the term molecular and just refer to Ring.

Section 2.2.1, p9214, line 9: There is an explanation for selecting the lower limit of the fitting interval, but nothing is said about the upper limit.

Our answer to the previous point already includes the discussion about why choosing the end of the fitting interval at 356 nm.

Section 2.2.1, p9215, line 7: Please explain the meaning of molecular Ring.

We refer here to the answer given two questions above.

Section 2.2.1, p9215, line 17: Please comment on the added value of using to closure polynomials instead of one (baseline and scaling, as called in table 1).

It allows us to disentangle different ways in which broad spectral features appear in our model of radiances.

Section 2.2.1, p9216, line 11: How do you define and estimate the detection limit?

Our answer to the first specific comment answers this question.

Section 2.2.2, p9216, line 18-19: please explain how gas concentrations are taken into account in AMF calculations. It is stated later that O3 profile variations are considered. Please explain how it is done.

We compute scattering weights using 26 ozone profiles from the TOMS v7 climatology. Despite having this information available we haven't implemented yet their dependency with the ozone total column. To give a broad description of the dependencies of w(z) we mention O_3 but later on we don't extend on its treatment because we haven't implemented it yet. Probably the source of confusion here is this sentence "w(z) are functions of the geometry of the observation (SZA, viewing angle (VZA) and relative azimuth angle (RAA)), the latitude, the O_3 profile, since it has the most significant absorption features, the aerosol load, the surface properties (reflectance and altitude) and the characteristics of the clouds present in the scene if any (cloud fraction and cloud pressure). " Since we don't have implemented this dependency yet in our code we propose to remove the reference to the O_3 .

Section 2.2.2, p9216, line 19: the surface height and reflectivity of the spatial pixel?

We have added the following text to clarify which surface characteristics are consider for each spatial footprint pixel.

"..., the characteristics of the spatial pixel footprint (surface reflectance and terrain height), and the geometry of the retrieval."

Section 2.2.2, p9217, line 20: A number is given for the variation of w(z) with wavelength (<7%). Please specify at which altitude z, or if it rather corresponds to a variation of the total AMF, and in this case, for which H2CO profile?

We refer here to the variation of the total AMF. We used a sample of profiles over Central Africa, South East US, the Amazon Basin, and the Pacific Ocean. We have modified the text as follows:

"Given the small variation of the AMF within the fitting window interval (usually less than 7%) we are calculating it at one wavelength (λ), 340 nm, which we consider representative of their mean value within the fitting window."

Section 2.2.3, p9218, line 24: Please define ΔVCD. I guess ΔSCD/AMF.

We have added the following text to clarify:

"Figure 4 shows ΔVCDs (defined as ΔSCD/AMF),..."

Section 3, p9220, equation 7: please define m and n.

We have added the following text in p9219 line 10:

"... freedom (m is the number of spectral points and n the number of fitted variables)."

Section 3, p9220: The sensitivity test on the profile shape is not clear. What is meant by a 10% bias of the profiles? Changing the total H2CO concentration of the a priori profile should not have any impact on the AMF. But varying the only surface concentration can change the AMF by much more than 16%. Please develop.

Referee 2 raised the same issue. We have changed the text as follow to clarify how we carried on the sensitivity analysis for H₂CO profiles:

Page 9220 lines 3 to 6:

"To estimate the error associated with AMF calculations we have performed a sensitivity analysis by perturbing one at the time the input parameters of AMF calculations. The parameters considered are cloud parameters, surface reflectance, terrain height and GEOS-Chem climatological profiles as well as the wavelength dependency of w(s) with in the fitting window. The amplitude of each perturbation is reflecting the uncertainties reported in the literature for each one of the parameters. A shortcoming of this method is that it assumes that errors due to different parameters are not correlated."

Page 9220 lines 19 to 24:

"To finish the sensitivity analysis of the AMF calculation we tested the impact of the a priori profiles of H_2CO . Since it is the shape of the profile what affects the AMF calculation we have applied the reported uncertainty only to layers showing the highest VMRs, defined as those that contribute to the 90% percentile. GEOS-Chem biases with respect to in situ measurements vary around the globe. For example over the US, GEOS-Chem simulations have biases of around 10% (Millet et al., 2006) which translate in AMFs uncertainties up to 16%. Over tropical regions Barkley et al. (2011) reported biases of up to 25% which translate in 40% AMFs uncertainties.

Considering the contributions from all these factors we estimate ε_{AMF} to be between 38%, for an optimistic case with small GEOS-Chem profile uncertainty and cloud parameters being the most significant source of uncertainty, to 50% when surface reflectance and GEOS-Chem profile uncertainties are at their maximum becoming significant sources of AMF uncertainty that contribute as much as the uncertainty in the cloud parameters."

Section 3, p9220, line 23: The final estimation of 38% is only valid for one particular observation condition, and it would be more insightful to provide a range of uncertainties, and the conditions in which the AMF errors are the largest/lowest. Alternatively, a figure showing the calculated error could be added to the figures 3 and 4, since an equation (equ. 7) is provided.

See answer provided for the previous comment.

Section 4, p9221, line 10: Please refer to De Smedt et al. (2015) for the BIRA OMI product.

Changed reference.

Section 4, p9222, line 8: Please check if version 14 of the BIRA product has been used. Differences can be significant between v13 and v14 over Southern Africa.

Thanks a lot for pointing this out. Obviously I was using version 13. I have updated figures 6, 7, 8, and the discussion in section 4. We have also had the opportunity to update the OMPS retrieval with the latest version of the cloud product. Therefore we have changed the discussion in section 4 quite significantly. Here is the text as it will be now:

".... The difference between the BIRA and SAO retrievals over the Pacific Ocean is induced by the underlying difference of the chemical transport models used for the reference sector correction. As expected, the differences between OMI BIRA and OMPS retrieval are greater than those between OMI SAO and OMPS. The absolute mean offset between OMPS SAO and OMI BIRA is 28% while it is 23% between OMI SAO and OMPS SAO.

While these mean absolute offsets give us an idea of how close the retrievals ae from a general perspective it is more interesting to consider the differences for particular regions. The most evident differences between OMI BIRA and OMPS, easy to appreciate in Figure 7, happen for the winter months over Southeastern US and Europe. For example in December over Southeaster US the bias between OMI BIRA and OMPS is -32%. The same month over Europe the differences are -15% between OMI BIRA and OMPS and 63% between OMI SAO and OMPS. Particularly over Europe it is important to consider the increased difficulty if the retrieval due to the viewing geometry (SZA and VZA) during that particular time of the year.

With few exceptions (winter months over Southeastern US, Europe and East China) retrieved H₂CO VCDs using OMPS are higher than columns retrieved using OMI as shown by the dominant blue color in Figure 7. This shows the bias between OMPS and OMI retrievals as the percentage of OMI minus OMPS. It is clear that to obtain a better idea of the accuracy of the different retrievals independent validation studies like the one recently published by Zhu et al. (2016) are needed. In this paper H₂CO satellite products produced by different groups using different instruments are compared with in situ measurements. The products included in this comparison are BIRA OMI, GOMA2A, and GOME2, SAO OMI, and OMPS and NASA Goddard OMPS. SAO OMPS retrievals are found to be bias 39% low over the Southeaster US between 5 August and 25 September 2013".



This are the updated figures:

Section 4, p9222, line 21: Considering the respective spectral and spatial resolutions of OMI and OMPS, the noise level of the OMPS retrievals should be lower than OMI. This needs to be discussed in the paper. I'm not sure that "the averaged VCDs variability considering all regions and months" give any information about the precision of the product. The variability of background values (Pacific Ocean) is generally used to estimate the precision, and should correspond to $\epsilon_{\Delta SCDrandom}$.

It is not our intention to provided information here about the precision of the products by providing these values. Our only intention is to show that different products may be capturing the structure with a region in different ways. It an information that the final user of satellite products should consider in each study based in their previous knowledge of the expected variation for a particular region.

Referee 2 ask to include a figure showing individual orbits for OMPS and OMI to better compare pixel size. This is now figure 5 and the text that makes reference to the increase of SNR due to OMPS lower spatial resolution. Page 9221, line 18: "... difference in the spatial pixel size. Figure 5 shows an almost coincident OMPS and OMI Africa overpass to better illustrate the differences in the pixel size. OMI has a nadir pixel of 24 x 13 km The apparent reduction of noise in OMPS retrievals in comparison with the OMI retrievals shown in Figure 5 is a direct consequence of OMPS lower spatial and spectral resolution which translate in SNR increases.

Conclusion, p9223, line 6: This sentence is in contradiction with the numbers given in section 4 (see comment just above). Besides, please consider the fact that if the detection limit numbers are weighted by the square root of the respective pixel areas (50x50 or 13x26), then the OMI detection limit is twice lower than OMPS.

See answer to previous question.

Conclusion, p9224, line 5: Please mention TROPOMI/S5P, to be launch in 2016.

Added.