Response to reviewers

We thank the reviewers for their comments. Below are our responses in blue.

In the course of responding to the reviewers, two main changes occurred: (1) a trend discussion was added and (2) we emphasize the lack of MLS penetration below the upper troposphere throughout the paper.

Trend discussion

Before the conclusions the following paragraphs will be added:

As an example, Figure 8 shows the H_2O and O_3 trends in the tropics computed using monthly zonal mean deseasonalized anomalies of the raw model fields, as well as using all the available satellite-sampled measurement locations and only those passing the screening criteria in the tropics. As shown, when all available measurement locations are used, the MIPAS and MLS sampling allows accurate derivation of trends, with values matching those calculated from the raw model fields almost exactly. However, when only those measurements passing the screening criteria are used, both instruments have limitations: MIPAS trends are impacted because of the large percentage of measurements screened out below 100 hPa, which introduces non-negligible artifacts (up to 80% change for H_2O and up to 20% change for O_3); MLS trends are impacted because of the reduced vertical resolution, which limits its usefulness to the upper troposphere and above. Note that the impact of quality screening on MIPAS trends can be mitigated by using a regression model similar to the ones used by Bodecker et al. (2013) and Damadeo et al. (2014). These models have been shown to mitigate the effects of the non-uniform temporal, spatial and diurnal sampling of solar occultation satellite measurements. Furthermore, MIPAS trend analysis can be restricted to regions less affected by deep convection (for example, the mid tropical Pacific) to minimize the quality screening effects.

The estimated number of years required to definitively detect these trends is also shown in Figure 8. These estimates were computed assuming a trend model similar to the one described by Tiao et al. (1990), Weatherhead et al. (1998), and Millán et al. (2016), with a seasonal mean component represented by the monthly climatological means. As shown, with the MIPAS screened fields additional years are required for robust trend detection (up to ~150 years for H_2O and up to ~40 years for O_3 versus 50 years and 20 years, respectively, when all available measurements are used).

Similar analyses were performed for other latitude bands. Although the magnitude of the trends derived when using the MIPAS screened measurement locations was also impacted in these cases, no significant difference was found in the number of years required to detect such trends. In addition, no significant artifacts were found for HNO_3, CO or temperature for either the trend magnitude or the number of years required to detect such trends. Note that, when using real data, the effect of instrument noise upon trends will be negligible due to the vast number of MIPAS or MLS measurements associated with each monthly latitude bin. Drifts and long-term stability issues on these datasets [i.e., Eckert et al., 2014; Hubert et al., 2016; Hurst et al., 2016] will have to be corrected.

In the conclusion section, the trend discussion will be changed to:
These biases affect trends derived from these measurements using a simple regression upon monthly zonal mean data substantially affected by clouds. Further, the number of years required to detect such trends may increase due to the extra noise added to the time series by screening out measurements.

The following figure will be added (as figure 8 of the revised paper):

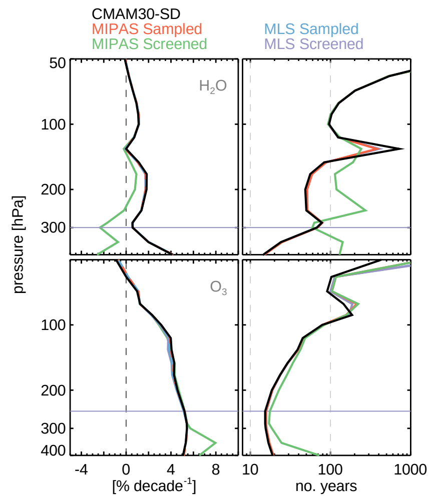


Figure 8: (left) H_2O and O_3 trends computed based on monthly zonal mean deseasonalized anomalies for the tropics (20S to 20N) using the raw model fields, all the available satellite measurements (MIPAS or MLS sampled) and only those measurements passing the screening criteria (MIPAS or MLS screened). Note that for O_3, we only use data starting from 2000 to capture the expected period of O_3 recovery. A purple line indicates the bottom (largest pressure) of the recommended range of the MLS retrievals. (right) Number of years required to detect such trends.

References:

Bodecker et al 2013: 10.5194/essd-5-31-2013
Damadeo et al 2014: 10.5194/acp-14-13455-2014
Tiao et al. (1990): 10.1029/JD095iD12p20507
Weatherhead et al. (1998): 10.1029/98JD00995
Millán et al (2016): 10.5194/acp-16-11521-2016

Lack of MLS penetration

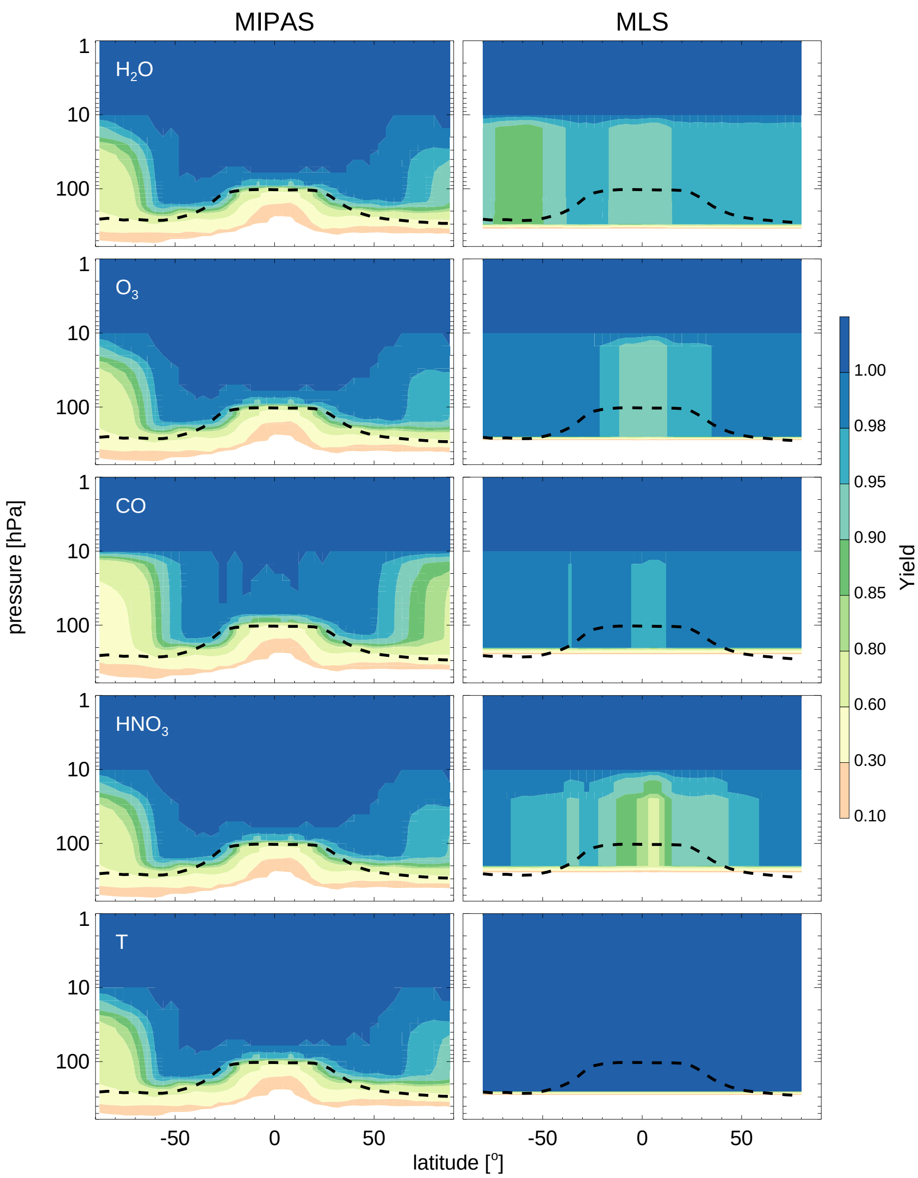
To emphasize more the MLS caveat, the sentence in P1L16 (in the abstract) will be changed to: In contrast, MLS data quality screening removes sufficiently few points that no additional bias is introduced, although its penetration is limited to the upper troposphere while MIPAS may cover well into the mid troposphere in cloud-free scenarios.

In P5 L8 this sentence will be changed: In contrast, in general MLS yield values are better than 90%, although the measurements do not extend below the upper troposphere.

In a similar manner P7 L18 will be changed to: However, continuum absorption in the microwave suppresses signals from the mid and lower troposphere in a limb viewing geometry, limiting the MLS vertical range to the upper troposphere and above while MIPAS may cover well into the mid troposphere in cloud free scenes.

And in the new paragraph about trends we included: However, when only those measurements passing the screening criteria are used, both instruments have limitations: MIPAS trends are impacted because of the large percentage of measurements screened out below 100 hPa, which introduces non-negligible artifacts (up to 80% change for H_2O and up to 20% change for O_3); MLS trends are impacted because of the reduced vertical resolution, which limits its usefulness to the upper troposphere and above.

Furthermore, we noticed that the Figures were not displaying the correct MLS pressure cut off. The revised versions showcase much better the lack of MLS penetration (as an example, the updated Figure 2 is shown below). Also, we superimpose a mean thermal tropopause derived from MERRA2 to Figure 2, 3, and 4.



Updated Figure 2

Reviewer 1 comments

This paper discusses the impact of non-uniform sampling of the MIPAS and MLS instruments on resulting zonally averaged data with particular emphasis on how data quality screening exacerbates biases. The authors describe how MIPAS and MLS have similar sampling biases but how MIPAS data is detrimentally affected by screening through the use of running MIPAS and MLS sampling through the CMAM30-SD CCM. While the methodology applied has some use and accurate in its basic conclusions, some of the more meaningful conclusions (e.g., impacts on ability to derive trends from different instruments in the UTLS) are not supported by analysis and thus speculative. Furthermore, the scope of this work is severely limited and the tone of the paper is seemingly self-serving. As such, I would recommend this work for publication only after additional work and major revision.

Major Comments:

Pg. 02, Line 29: "We emphasize that the results of this study refer only to the representativeness of the respective data, not to their intrinsic quality." This statement greatly detracts from the value of this work. This work makes very clear remarks regarding the impact of sampling biases on the ability to use certain kinds of data sets for trend analysis in the UTLS and how sampling biases will require longer data sets because of the added noise. However, the quality of the data sets that are used is a critical component to those kinds of analyses. Recent work in the 2014 Ozone Assessment or the SI2N effort (https://www.atmos-chem-phys.net/ special_issue284.html) have shown that sampling biases, while present in trend analyses, are not necessarily the greatest driver of trend uncertainty as data quality issues and instrument drifts are also present. Incorporating data quality into the calculation is necessary, as it is still possible for higher precision data with sampling biases to be more robust for trending work than lower precision data, though it ultimately depends on what those precisions and sampling impacts are.

This will be expanded to: We emphasize that the results of this study refer only to the representativeness of the respective data, not to their intrinsic quality. Their quality has been extensively evaluated in numerous data characterization and validation papers [i.e., Pumphrey et al., 2007; Read et al., 2007; Santee et al., 2007; Schwartz et al., 2008; Stiller et al, 2012; Hegglin et al., 2013; Raspollini et al, 2013; Neu et al 2014; Livesey et al., 2017; Sheese et al., 2017]. Furthermore, their long-term stability has also been studied [i.e., Nair et al., 2012; Eckert et al., 2014; Hubert et al., 2016; Hurst et al., 2016].

In addition, a new paragraph about trends will be added (see above) which will include the following sentence: Note that, when using real data, the effect of instrument noise upon trends will be negligible due to the vast number of MIPAS or MLS measurements associated with each monthly latitude bin. Drifts and long-term stability issues on these datasets [i.e., Eckert et al., 2014; Hubert et al., 2016; Hurst et al., 2016] will have to be corrected.

References:

Pumphrey et al. 2007: 10.1029/2007JD008723
Read et al 2007: 10.1029/2007JD008752
Santee et al 2007: 10.1029/2007JD008721
Schwartz et al 2008: 10.1029/2007JD008783
Nair et al 2012: 10.5194/amt-5-1301-2012
Eckert et al 2014: 10.5194/acp-14-2571-2014
Neu et al 2014: 10.1002/2013JD020822
Stiller et al, 2012: 10.5194/amt-5-289-2012
Hegglin et al 2013: 10.1002/jgrd.50752
Raspollini et al 2013: 10.4401/ag-6338
Hubert et al 2016: 10.5194/amt-9-2497-2016
Hurst et al 2016: 10.5194/amt-9/4447-2016

Sheese et al 2017: 10.1016/j.jqsrt.2016.06.026

Pg. 06, Line 32 and Pg. 07, Line 25: "These poor metrics imply that any trends derived at these pressure levels will also be impacted by quality screening induced biases: the magnitude of the trends will be affected because of the change in the slope, and the number of years of observations required to conclusively detect trends will considerably increase due to the noise associated with the worsening of the coefficients of determination (e.g., Millán et al., 2016)."

Biases and trends can be completely independent and the slopes that are referred to here are not trend slopes but correlation slopes. For example, a seasonally dependent dry bias in H2O as shown in Fig. 5 does not guarantee an induced bias in the trend values and so the impact of these sampling biases on trends is not directly addressed by this work. Furthermore, while it is true that increased noise in the data can result in requiring longer duration data records to determine significant trends, neither this study nor Millan et al. (2016) considers the attribution between data quality and non-uniform sampling. Without additional work to address the impacts of each of these factors, this entire statement is only speculative.

See discussion on trends above.

In general, the scope of this work is severely limited. The statement that an instrument's inability to see through clouds will result in less data is obvious while comparing two data sets to ascertain the impact on trends without considering data quality is neglectful. As it stands, this study has limited to no scientific value. However, the underlying concept of this work could be expanded albeit with simulated sampling and uncertainties. For example, the authors could simulate different sampling patterns from different orbit types and sampling frequencies for an expected limb sounder. Running these through model data would allow for comparisons of the impact of different potential sampling patterns. To further test potential data quality screening, utilizing model cloud fields or retrieval limitations of different observation techniques would create another variable to test rather than using the data quality screening of a specific instrument. Lastly, the authors could simulate differing data precisions or vertical resolutions from all of these sensitivity tests and incorporate the resulting uncertainties into trending analyses to determine the impact of all of these variables on the derived trends. This would provide a large solution space to test the impacts of potential measurement systems on their ability to be used for trending analyses in the UTLS region. While these suggestions are extensive and perhaps more comprehensive, some aspect(s) would be necessary to incorporate actual data quality into the authors' data quality screening to back up the claims regarding the impact on trend detection.

The main purpose of this study is to quantify the impact of screening biases using MIPAS and MLS as proxies for IR and MW limb sounder measurements, not to run a full Observing System Simulation Experiment (OSSE – the exercise the reviewer is essentially suggesting) to study different sampling patterns. That would make the paper much less focused. Furthermore, the MIPAS and MLS sampling patterns are so dense that the sampling bias is negligible for both (as shown here); that is, *the problem is not in the sampling pattern per se but rather in the inability to measure in cloudy scenes*, which leads to the "obvious" reduction in data. Hence no matter what sampling patterns are explored, the problem will still be there for IR based measurements. Furthermore, when dealing with real data, it will not only be a matter of the reduced number of measurements but also, the reduced representativeness of the average because clouds are correlated with the atmospheric state.

Moreover, an OSSE will require a threshold to determine which clouds affect the IR and the MW data. Such thresholds may be problematic to define and not actually useful in real-world scenarios. By using the screening applied to real data we circumvent this problem by using the criteria determined by the instrument teams to obtain the best data possible from their respective instruments.

Perhaps what is most troubling is the tone of the paper. It seems that the purpose of this paper is to act as a published reference for why a future MLS instrument must be used to ascertain long-term trends of trace gas species in the UTLS. The authors appear to go to great lengths to phrase the message as to assert the “superiority” of MLS measurements over MIPAS at every turn (i.e., pointing out all potential deficiencies in MIPAS data without mentioning any for MLS), and even go as far as attempting to undermine the usefulness of other current or future measurement systems as evidenced by the last two sentences in the paper. While this type of rhetoric is expected in a proposal, it is not suited for a scientific publication

We recognize the reviewer's concern, and hope that our changes detailed above (the inclusion of a discussion on the lack of MLS penetration), combined with our decision to delete the final sentence of the conclusion, alleviate them.

In addition, we will add in P4L5 (in the MIPAS IMK introduction): MIPAS IMK/IAA algorithm retrieves temperature and more than 30 species including O_3, H_2O, CO, CFCs, PAN, among many others.

Minor Comments:

Pg. 01, Line 23: “Further, satellite missions such as . . . have records that span more than a decade.” This statement is phrased in such a way as to suggest that no ground station data have records that long. I would suggest revising. The sentence will be changed to: Further, like many ground-based data sets, satellite mission such as …

Pg. 02, Line 09: “They concluded that coarse non-uniform sampling leads to nonnegligible biases . . .” Biases in what? Is that data biased from the sampling or are the analysis methods not conducive to using data with non-uniform sampling? The sentence will be changed to: They concluded that coarse non-uniform sampling leads to non-negligible zonal mean biases.

Pg. 02, Line 13: “They found that coarse non-uniform sampling patterns can induce significant errors in the magnitudes of inferred trends . . .” Again, is this a flaw in the data or the analysis method? This will be changed to: They found that coarse non-uniform sampling patterns can induce significant errors in the magnitudes of trends inferred directly from monthly zonal means, …

Pg. 04, Line 12: “MLS measures around 3500 vertical scans daily, providing nearglobal (82S to 82N) observations.” Please also include the geospatial sampling characteristics of the MIPAS instrument in its description. It is in P3 L22 of the original manuscript “MIPAS measured around 1350 vertical scans daily, providing global observations.” Thus, no changes have been made in the revised manuscript to address this comment.

Pg. 04, Line 20: "Further, we used the vertical grid of the CMAM30-SD fields; that is, we assume that MIPAS and MLS vertical resolution is good enough to resolve these model fields, at least in the upper troposphere / lower stratosphere (UTLS)." What are the vertical resolutions of the model and instruments in the UTLS?
The vertical resolution of the model is in the original manuscript (P3 L15). For MIPAS and MLS, the vertical resolution will vary by specie but overall, they are between 3 and 4 km. Taking this into account, the sentence will be changed to: Further, we used the vertical grid of the CMAM30-SD fields; that is, the impact of the vertical resolution of the measurements is not taken into account. However, note that, in this case, both instruments have similar vertical resolutions in the upper troposphere / lower stratosphere (UTLS), varying overall from 3 to 4 km.

Pg. 06, Line 31 and Pg. 07, Line 24: "The biases for O3 and HNO3 oscillate between -10. Unfortunately, we couldn't address this comment as it seems to us that it is incomplete.

Figure 5: It would be better to change the X-axis label interval on the time-series plot to every 5 years.
We changed it to every two years and increased the font size.

Figures 6 and 7: There is a lot of unnecessary white space in some of these plots, though given the desire to maintain consistent axes ranges between the two I can see why Figure 6 has so much white space. That having been said, I still think some reductions can be made to make the results easier to see.
The x-ranges have been reduced as much as they can be without cutting out any of the lines shown.

Additionally, for whatever reason the line thicknesses appear the same between Figs. 6 and 7 when zoomed out but are much thinner in Fig. 6 when zoomed in. They will be the same thickness in the new version.

Lastly, what is the bottommost pressure level on the Y-axis?
The bottommost level and the top pressure level are 400 and 50 hPa, these levels will be added to the figures.

Reviewer 2 comments

The paper is dedicated to the characterization of sampling biases in infrared and microwave limb sounding instruments, with MIPAS and MLS taken as examples. The paper is a continuation of a series of publications on characterization of sampling biases. The new aspect is analyzing the influence of quality screening on data representativeness.

MAJOR COMMENTS

1) It is stated in the abstract that " analysis of long-term time series reveals that these additional quality screening biases may affect the ability to accurately detect upper tropospheric long-term changes using such data" (similar statements are on page 6 and in conclusions) However, the performed analyses are insufficient for such statement. It is rather expected that the screening of cloudy conditions results in biased estimates, and that the variability might not be represented properly. However, biased estimates, not perfect correlation coefficient with the full time series and R2 do not necessary imply that the long-term trends are inaccurate. Furthermore, if the sampling patterns do not change over time, a large part of sampling uncertainty can be removed in the trend analysis by consideration of deseasonalized anomalies. In order to make such statement on ability of accurate trend detection, the authors should perform trend analysis using the full and sub-sampled datasets and support their statements by quantitative estimates. Another, a simpler solution, is to remove these abovementioned statements on ability to accurately detect trends from the manuscript.

See discussion on trends above.

If the authors will decide to extend the analyses, it would be also interesting to investigate the influence of sampling patterns on ability to reproduce the natural cycles.

We decided not to expand the manuscript upon the ability to reproduce natural cycles because we believe that is outside the scope of the current paper.

2) The value of the paper will be increased significantly, if the presented analyses of sampling biases using the modelled data are enhanced with comparison of real experimental data from MIPAS and MLS. Such analyses would illustrate whether the observed biases are explained by sampling patterns.

After careful consideration, we decided not to include a comparison of the real data, because such comparisons will suffer from the fact that we do not know the truth and because such comparisons can be found in several validation papers. The fact that extensive validation of these data sets has been documented in previous validation papers is now noted in the revised manuscript.

MINOR COMMENTS

1) P.4, L.5 : Please write the version of the IMK/IAA processor. We will add: in particular version 5.

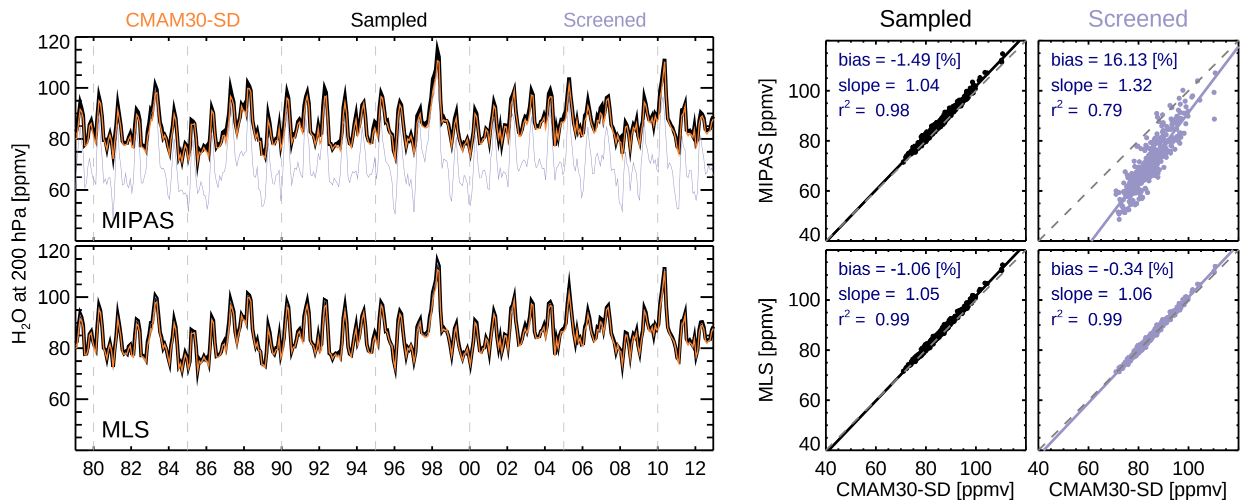
2) P.2 L.11: The sampling uncertainty has been also discussed in (Sofieva et al., 2014). In this paper, the authors analysed the sampling biases for 6 satellite instruments and proposed a parameterization of sampling uncertainty in monthly zonal mean data.

Sofieva, V. F., Kalakoski, N., Päivärinta, S.-M., Tamminen, J., Laine, M. and Froidevaux, L.: On sampling uncertainty of satellite ozone profile measurements, Atmos. Meas. Tech., 7(6), 1891–1900, doi:10.5194/amt-7-1891-2014, 2014. 3)

We will modify that section as follows: For the limb sounding technique, Sofieva et al., (2014) estimated the sampling biases in zonal mean ozone profiles from six limb-viewing satellite instruments and proposed a simple parameterization to estimate them. Toohey et al., (2013) characterized the sampling bias for H_2O and O_3 …

Figure 5: Please use more distinct colors in scatter plots.

The colors were changed, see below:



The caption will be changed accordingly: The dashed gray lines are the 1:1 line, and the solid lines are the linear best fits, whose slopes are given.

Reviewer 3 comments

The paper by Millan et al. describes effects of sampling and quality screening for two limb sounding instruments (MLS and MIPAS). Based on CCM data the analysis shows significant biases in the zonally averaging of various trace gases and temperature distribution, especially for a MIPAS-like instruments with its cloud-induced quality screening. Biases in the zonal means as well as for trend analyses in the upper troposphere can be quite large, which is an important fact and needs consideration in any trend analysis.

General comments:

There are two major concerns regarding the manuscript from Millan et al.:

a) The study highlights a very specific caveat of sampling and screening issues of space borne instruments. The whole approach is very technical, investigating a very obvious problem of the IR limb measurements due to cloud screening, which can have a severe effect on the results especially if you like to analyse trends in the very cloudy upper tropical troposphere. Although this effect is of interest for ACP community, these kind of analysis is not really suited for ACP. The whole manuscript looks more like a technical study or a technical note (for example as prepared for NASA or ESA studies for future satellite sensors) and is not sufficient for a full publication in a journal like ACP. A more in-depth study of the MW/IR limb caveats on trend analyses cloud be publishable in a more technical and instrument orientated journal like Atmospheric Measurement Techniques.

As the referee notes, determination of trends is a critical issue of great current concern. While the effects of clouds on IR measurements are indeed well known, the impact of removing cloud-affected profiles on biases in zonal means and the trends estimated from them has not been quantified before. Hence, we believe that this paper is appropriate for ACP because its results directly impact the broad UTLS community.

b) To my mind, this paper does not contribute a substantial add-on to a former study of the authors. The paper by Millan et al. (2016) in ACP describes most of the general effects of sampling pattern, which can be quite similar effects to the quality screening, in the context of a much more detailed study on atmospheric trend analyses. My strong impression is that the actual manuscript misses new concepts and methods and just repeats parts of the Millan et al. (2016) analyses with another combination of satellite instruments.

The new addition is the quantification of the screening bias *on top of* the sampling bias. Previous studies (Toohey et al., 2013; Sofieva et al., 2014; Millán et al., 2016) focused on the sampling bias while disregarding the effects of data quality screening. As shown in Figure 3 and 4 of the paper, the effects of the screening biases are not insignificant and need to be known and quantified. A different combination of satellite instruments was essential to this study because the idea was to take data sets with comparable sampling biases and show how they diverge when screening biases are taken into account.

P2 L17 will be expanded: However, none of these studies have quantified the additional biases introduced through quality screening of the measurements, that is, this study isolates and quantifies another source of uncertainty in averaged data.

Major comments:

1) P4, line 29: Although the screening is a fundamental issue of the study, there are no details presented for MLS (but some for MIPAS). Please, at least summarize the main topics of Livesey et al. (2006). In addition, more details on the cloud screening of MIPAS would be helpful as well (see next comment).

We will add: The screening procedure applied to MLS data follows the guidelines detailed by Livesey et al. (2017): We only use data within the specified pressure ranges; we neglect profile points for which the precision is negative (which indicates that the retrievals are influenced by the a priori); we avoid profiles for which the "Status" field is an odd number (which indicates operational abnormalities or problems with the retrievals); and we only use profiles for which the "Quality" and "Convergence" fields are within the specified thresholds. The "Quality" field describes the degree to which the measured radiances have been fitted by the retrieval algorithm and the "Convergence" field is a ratio of the fit achieved at the end of the retrieval process to the value predicted at the previous step.

2) P5, line 1: Please note somewhere here that the MIPAS cloud-screening applied in the IMK product is a very conservative approach with respect to cloud effects in the measured spectra. This might have effects on the presented analysis. Especially, in the tropical upper troposphere high water vapour abundance will result in false-positive cloud detections (e.g. Spang et al. 2012) in the IMK product and consequently an artificial overestimation in the biases, where other MIPAS level 2 processors might do a better job. This objective should be addressed in the manuscript.

The following sentence will be added in P5 line 28: We note that the cloud screening procedure of the IMK/IAA algorithm is conservative with respect to those of other MIPAS processors [Spang et al., 2012]. On the face of it, it appears that this causes an unnecessarily large sampling bias which could be avoided by using a less restrictive cloud screening threshold value. The purpose of a conservative cloud screening procedure is to guarantee that the measurements passing the cloud screening are indeed unaffected by any cloud signal in the spectra. Cloud signals can lead to systematic retrieval errors, which are correlated to the state of the atmosphere, hence, the sampling biases would merely be replaced by retrieval biases. This, we think, is worse, because then both the parent data and the zonal averages would be affected, while with a conservative screening only the averages are affected but not the parent data which survive the screening.

3) The disadvantages of the cloud screening in the tropical UT for the IR measurements are highlighted frequently in the manuscript and are presented by different types of analyses, but with only very limited further information content. In contrast, the caveat of MW sounders to retrieve trace gases below ~300 hPa at any latitude is only briefly mentioned. Studies for future ESA missions, like the PREMIER report for mission selection (http://projects.knmi.nl/capacity/PREMIER/SP1324-3_PREMIERr.pdf), show nicely the excellent synergy by a combination of IR and MW (s. Fig. 4.2 of the report), where IR-limb still allows measurements in the mid-troposphere, where MW-limb fails to measure.

See MLS lack of penetration section above.

4) To my mind the trend analysis section needs to be improved. Although MIPAS tackles to deliver good trend analyses in tropical UT, this is a shortened result. Have you tested if the biases are better, if the

trend analyses are restricted to longitude regions where convection is less pronounced (e.g. mid-Pacific, Atlantic regions, excluding the warm pool region, central Africa and South America, where deep convection and cloud-coverage is most pronounced). Local trends in the UT/MT in tropical and subtropical areas would be valuable in principle.

See trends section above.

The reviewer is correct in pointing out that trends restricted to longitude regions where convection is less pronounced will be less affected (or barely affected) by cloud screening biases. For example, the following figure shows the yield at 200hPa for MIPAS and MLS water vapor and O_3 as well as the trends computed in the mid-Pacific where the MIPAS yields are less affected. As can be seen, the impact of the quality screening upon the trends in these region is minimal. In the paper we will add: Furthermore, MIPAS trend analysis can be restricted to regions less affected by deep convection (for example, the mid tropical Pacific) to minimize the quality screening effects.

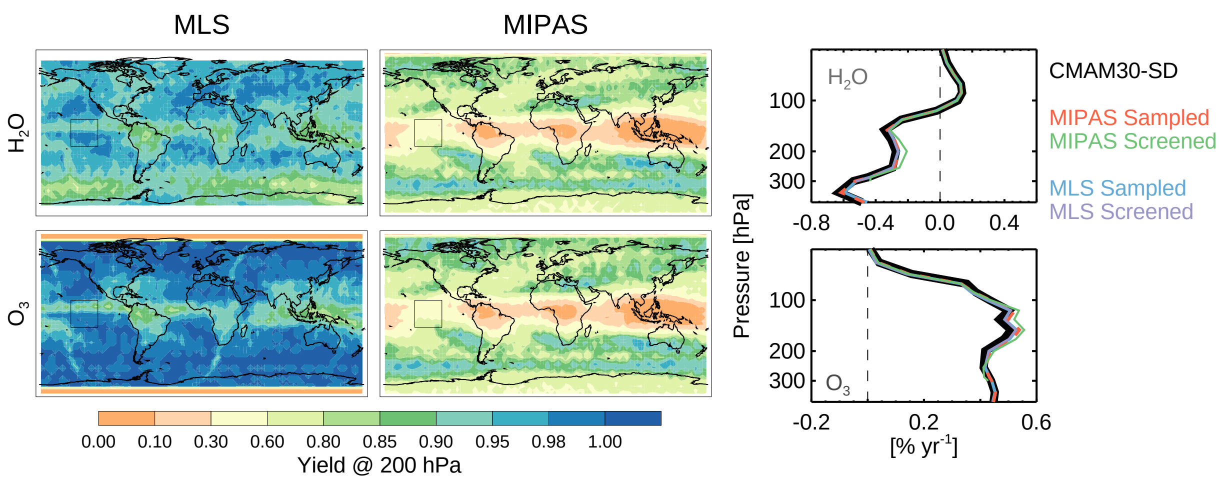


Figure: (right) Yield maps, (left) trends computed in the mid-pacific area shown in the maps for O_3 and H_2O.

5) I am also wondering why the authors argue that most of the biases are not caused by a lack of observations in convective (cloudy) areas in the tropics but are caused by a reduction in the overall sampling number. I think this is linked with each other, especially for water vapour with its extreme vertical and horizontal gradients. This objective would need further investigations for a final publication and is not sufficiently discussed by the only two sentences in section 3 (p5, line 25).

The sentence will be expanded as follows:
Although this resembles the expected dry bias in clear-sky tropospheric infrared measurements (e.g., Sohn et al., 2006; Yue et al., 2013) — that is, the fact that infrared instruments cannot measure cloudy regions where H2O is high, resulting in a dry bias — **the biases shown here are due to a combination of two factors: (1) high H2O values associated with deep convection** (**the screened-out locations might not necessarily be cloudy in the model fields however they are for the most part in the tropics, in regions of high H2O values, see Figure 1 for an example) and (2) due to the reduced sampling frequencies.** Note that this also applicable to other parameters …

6) Further, the quantification of the number of years needed to compensate for the biases introduced by the intensive cloud-clearing for IR limb sounder, which is only briefly mentioned in the Summary and Conclusion section, would be a very interesting topic for more detailed analyses and would improve the quality of the manuscript.

See trends section above.

Minor comments:

1) P2, line 23: Please, add a reference. We will add: [e.g., Livesey and Read (2000), Carlotti et al. (2001, 2006), Kiefer et al. (2010), Castelli et al. (2016)].]

References:
Livesey and Read (2000) - 10.1029/1999GL010964
Carlotti et al (2001) - 10.1364/AO.40.001872
Carlotti et al (2006) - 10.1364/AO.45.000716
Kiefer et al (2010) - 10.5194/amt-3-1487-2010
Castelli et al (2016) - 10.5194/amt-9-5499-2016

2) P3, line 3: Have you introduced CMAM30-SD already? We will change it to: CMAM30-SD (the Canadian Middle Atmosphere Model run in Specified Dynamics mode) is a coupled chemistry climate model nudged to the winds and temperatures of the ERA-Interim reanalysis…

3) P4, line 7: Please, explain in more detail, why the horizontal gradients are that important and why a different retrieval scheme might fail.
The following text will be added: Horizontal gradients are important because the line of sight extends around a thousand kilometers, crossing situations where the assumption of horizontal homogeneity is unrealistic (i.e., 1D retrievals). Several studies have discussed the advantages of including inhomogeneities along the line of sight for atmospheric retrievals [e.g., Livesey and Read (2000), Carlotti et al. (2001, 2006), Kiefer et al. (2010), Castelli et al. (2016)].

References:
Livesey and Read (2000) - 10.1029/1999GL010964
Carlotti et al (2001) - 10.1364/AO.40.001872
Carlotti et al (2006) - 10.1364/AO.45.000716
Kiefer et al (2010) - 10.5194/amt-3-1487-2010
Castelli et al (2016) - 10.5194/amt-9-5499-2016

4) P4, line 12: Are the ice cloud properties retrieved by a tomographic approach as well? Is a 2D or 3D tomographic approach, this should be mentioned.
The ice retrieval is not tomographic but rather 1D. The large degree of spatial inhomogeneity in cloud amount and cloud properties make tomographic retrieval approaches unstable in many situations, necessitating a simpler "1D" cloud retrieve whereby each limb view is considered to represent an independent cloud scene. The sentence will be changed to: These radiances are inverted using a 2D

tomographic optimal estimation algorithm (Livesey et al., 2006) that allows the retrieval of temperature and composition.

5) This paper highlights technical aspects of the two sensors, so it might be helpful to include a minimum of instrumental details like field of view (FOV), vertical sampling (step size), retrieval resolution, and horizontal sampling. Otherwise the reader cannot judge on statements like 'the vertical resolution is good enough to resolve these model fields' without any reference.
We decided not to include details about FOV, vertical sampling, etc, so as not to confuse the reader with too many details about the measurements when this paper is actually using interpolated fields. Note that the vertical resolution of the model is in the original manuscript (P3 L15). The statement the reviewer refers to was changed to: Further, we used the vertical grid of the CMAM30-SD fields; that is, the impact of the vertical resolution of the measurements is not taken into account. However, note that, in this case, both instruments have similar vertical resolutions in the UTLS varying overall from 3 to 4 km.

6) Figure 1: please give some details why MIPAS fails to retrieve the most northern profiles. This looks like an artefact of the data processing. I would not expect strong horizontal gradients or clouds at these locations, like argued in the manuscript. Why fails MLS retrieval at some high northern latitudes as well? You should explain in more detail in the manuscript why and where retrieval my fail for both instruments.
An investigation of why both retrievals fail in those areas is outside the scope of this study.

7) Figure 3: Any explanation for the cold bias in the area of the south-pole for MIPAS? This is a bit confusing, because especially in the cold areas PSC are frequent and hamper proper retrievals for this part of the season, consequently I would expect a warm bias?! That would be assuming that CMAM30SD properly behaves in those regions, which may not be the case, further, this might be just a random effect due to sparse sampling after screening out the measurements.

Technical comments:

1) Figure 2, 3, and 4: A superimposed mean tropopause location will substantially improve the information content of the figures around the tropopause.
We will superimpose a mean 2005 thermal tropopause derived from MERRA2. See updated figure 2 above for an example.

2) Figure 2: please, give a few more details in the figure caption. E.g. Za-Zr or Zr-Za? We will add in brackets: N_{QS} / N_A where N_A is the number of measurements available and N_{QS} is the number of measurements left after applying the quality screening criteria.

3) Figure 5: The numbers on the x-axis are not well readable and should be sparser and separated. We changed it to every two years and increased the font size.

4) Figure 6+7: Temperature biases should be presented with a scaling of T (e.g. K x 10). Then the significant temperature bias in the tropics will become more obvious. In addition, a tropopause location might help here as well. The temperature biases will be shown as Kx10. We will change the x-label to [% or K*10] and the average climatological tropopause value for that latitude bin will be shown as a dashed black line.

The caption of figure 6 will be changed to: Vertical profiles of the coefficient of determination, the bias, and the linear fit slope for different latitude bands for the MIPAS vs CMAM30-SD scatter using the full satellite-sampled fields. Note that for clarity the temperature bias is shown as K*10. Blue, green, red, purple, and orange lines represent H_2O, O_3, CO, HNO_3, and temperature metrics. The dashed black lines show the mean 2005 thermal tropopause derived from MERRA2 for the particular latitude bands.

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Characterizing Sampling and Quality Screening Biases in Infrared and Microwave Limb Sounding

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Abstract. This study investigates orbital sampling biases and evaluates the additional impact caused by data quality screening for the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) and the Aura Microwave Limb Sounder (MLS). MIPAS acts as a proxy for typical infrared limb emission sounders, while MLS acts as a proxy for microwave limb sounders. These biases were calculated for temperature and several trace gases by interpolating model fields to real sampling patterns and, additionally, screening those locations as directed by their corresponding quality criteria. Both instruments have dense uniform sampling patterns typical of limb emission sounders, producing almost identical sampling biases. However, there is a substantial difference between the number of locations discarded. MIPAS, as a mid-infrared instrument, is very sensitive to clouds, and measurements affected by them are thus rejected from the analysis. For example, in the tropics, the MIPAS yield is strongly affected by clouds, while MLS is mostly unaffected.

The results show that upper tropospheric sampling biases in zonally averaged data, for both instruments, can be up to 10% to 30%, depending on the species, and up to 3 K for temperature. For MIPAS, the sampling reduction due to quality screening worsens the biases, leading to values as large as 30% to 100% for the trace gases and expanding the 3 K bias region for temperature. This type of sampling bias is largely induced by the geophysical origins of the screening (e.g. clouds). Further, analysis of long-term time series reveals that these additional quality screening biases may affect the ability to accurately detect upper tropospheric long-term changes using such data. In contrast, MLS data quality screening removes sufficiently few points that no additional bias is introduced, although its penetration is limited to the upper troposphere while MIPAS may cover well into the mid troposphere in cloud-free scenarios. We emphasize that the results of this study refer only to the representativeness of the respective data, not to their intrinsic quality.

1 Introduction

Satellite limb sounders have provided a wealth of information for studies affecting climate, ozone layer stability, and air quality, as well as evaluation of reanalyses and chemistry climate models. Compared to ground-based instruments or aircraft field campaigns, satellite data provides continuous coverage over large areas (or even global scales, depending on their sampling), facilitating model evaluation on a large scale. Further, like many ground-based data sets, satellite missions such as the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) (Bernath et al., 2005) and the Aura Microwave Limb Sounder (MLS) (Waters et al., 2006) have records that span more than a decade. In addition, data records constructed using several satellite instruments that span more than 3 decades (Froidevaux et al., 2015; Davis et al., 2016) provide the opportunity to study and evaluate long-term variability and trends. However, satellite observations sample the continuously changing atmosphere only at discrete locations and times, which can result in a biased depiction of the atmospheric state.

Several studies have evaluated the impact of orbital sampling by comparing raw model fields against satellite-sampled ones (e.g., McConnell and North, 1987; Bell and Kundu, 1996; Engelen et al., 2000; Luo et al., 2002; Brindley and Harries, 2003; Aghedo et al., 2011; Guan et al., 2013). For the limb sounding technique, Sofieva et al. (2014) estimated the sampling biases in zonal mean O_3 profiles from six limb-viewing satellite instruments and proposed a simple parameterization to estimate them. Toohey et al. (2013) characterized the sampling bias for H_2O and O_3 for 16 satellite instruments, including limb scattering sounders, solar and stellar occultation instruments and limb emission sounders. They concluded that coarse non-uniform sampling leads to non-negligible zonal mean biases, not only through non-uniform spatial sampling but mostly through non-uniform temporal sampling, that is, producing means using measurements that span less than the full period in question. Millán et al. (2016) studied the sampling bias for temperature and several trace gas species for a subset of the instruments used by Toohey et al. (2013) and investigated the impact of such biases upon stratospheric trend detection. They found that coarse non-uniform sampling patterns can induce significant errors in the magnitudes of trends inferred directly from monthly zonal means, necessitating analysis of considerably more years of data to conclusively detect a trend. In contrast, dense uniform sampling patterns accurately reproduce the magnitude of the trends, with the number of years of data required determined mostly by natural variability.

However, none of these studies have quantified the additional biases introduced through quality screening of the measurements, that is, this study isolates and quantifies another source of uncertainty in averaged data. Many of the measurements discarded through quality screening have been affected by the presence clouds, which pose a substantial challenge to limb observations as the long limb path traverses hundreds of kilometers. The impact of such cloudy scenes depends on the measurement technique used. For example, instruments measuring microwave emission are unaffected by all but the largest particles in the thickest clouds. Many other limb measurements are screened out because of temperature gradients near the poles, whose impact varies depending on the retrieval scheme, i.e., one dimensional versus tomographic, as well as how accurately the a priori or initial guess captures such gradients (e.g., Livesey and Read, 2000; Carlotti et al., 2001, 2006; Kiefer et al., 2010; Castelli et al., 2016).

This study examines the sampling bias and quantifies the impact of quality screening upon two limb viewing instruments, one using microwave emission (the Aura Microwave Limb Sounder - MLS) and the other one using infrared emission (the ENVISAT Michelson Interferometer for Passive Atmospheric Sounding - MIPAS). Both instruments have dense uniform sampling distributions, which should minimize the sampling biases; however, there is a substantial difference in the number of measurements rejected through quality screening for these techniques (see Figure 1). The discarded profiles tend to cluster geophysically, leading to biases in analyses that are based on the remaining measurements. We emphasize that the results of this study refer only to the representativeness of the respective data, not to their intrinsic quality. Their quality has been extensively evaluated in numerous data characterization and validation papers (i.e., Pumphrey et al., 2007; Read et al., 2007; Santee et al., 2007; Schwartz et al., 2008; Stiller et al., 2012; Hegglin et al., 2013; Raspollini et al., 2013; Neu et al., 2014; Livesey et al., 2017; Sheese et al., 2017). Furthermore, their long-term stability has also been studied (i.e., Nair et al., 2012; Eckert et al., 2014; Hubert et al., 2016; Hurst et al., 2016).

2 Data and Methodology

2.1 Model Fields

CMAM30-SD (the Canadian Middle Atmosphere Model run in Specified Dynamics mode) is a coupled chemistry climate model nudged to the winds and temperatures of the ERA-Interim reanalysis. This nudging exploits the much better dynamics of the reanalysis to reliably predict the chemical fields. More information can be found in Scinocca et al. (2008), de Grandpré et al. (2000) and McLandress et al. (2014). Extensive validation (de Grandpré et al., 2000; Hegglin and Shepherd, 2007; Melo et al., 2008; Jin et al., 2005, 2009) has shown that the free-running version of this model performs well against observations relevant to dynamics, transport, and chemistry. Comparisons against ACE-FTS and the Odin Optical Spectrograph and Infrared Imaging System (OSIRIS) have shown that CMAM30-SD has a good representation of stratospheric temperature, H_2O, O_3, and CH_4 in polar regions (Pendlebury et al., 2015). Further, CMAM30-SD has been used to construct a long-term H_2O record, acting as a transfer function between satellite observations (Hegglin et al., 2014), and it reproduces halogen-induced midlatitude O_3 depletion sufficiently well to be used in long-term O_3 trend studies (Shepherd et al., 2014).

The CMAM30-SD version used in this study has a horizontal resolution of approximately 3.75°, that is, approximately 400 km (similar to the $\sim$500 km limb viewing path length). It has a lid at 0.0007 hPa with 63 vertical levels that vary from $\sim$500 m in the lower troposphere to $\sim$3 km in the mesosphere. Here, we present results using the H_2O, O_3, CO, HNO_3, and temperature CMAM30-SD fields. Note that for this study it is not necessary for the model fields to be correct in absolute terms. CMAM30-SD is simply used as a representative evolving atmospheric state.

2.2 Satellite Instruments

We analyze the impact of sampling and quality screening of the limb emission sounders MIPAS and MLS. MIPAS (Fischer et al., 2000, 2008) was launched in March 2002 on the European Space Agency Environment Satellite. MIPAS was a Fourier transform spectrometer conceived to record limb emission spectra. It covered the mid-infrared region from 685 to 2410 cm^{-1} in five spectral bands, allowing retrievals of temperature, pressure and trace gases. MIPAS measured around 1350 vertical scans daily, providing global observations.

From July 2002 to March 2004, MIPAS operated in full resolution mode, with a spectral spacing of 0.025 cm^{-1}; however, following persistent malfunctions with the interferometer slide mechanism, instrument operations were temporarily suspended. In January 2005 operations were resumed with MIPAS operating at a spectral spacing of 0.0625 cm^{-1}. This mode of operation is known as optimum resolution, and it is characterized by finer vertical and horizontal sampling attained through the degraded spectral spacing. MIPAS took quasi-continuous measurements until April 2012, when the European Space Agency lost contact with ENVISAT.

In the optimum resolution operation, MIPAS has several measurement modes: the nominal mode, with 27 tangent heights from 6 to 70 km; the middle atmosphere mode, with 29 tangent heights from 18 to 102 km; and the upper atmosphere mode, with 35 tangent heights from 42 to 172 km. The nominal mode covers the entire stratosphere extending into both the upper troposphere and the lower mesosphere to study linkages between these atmospheric layers. In this study we use the geolocations of this measurement mode because it covers around 80% of the measurement time (Fischer et al., 2008).

Several retrieval algorithms have been developed for the MIPAS spectra (e.g. Ridolfi et al., 2000; von Clarmann et al., 2003; Hoffmann et al., 2005; Carlotti et al., 2006; von Clarmann et al., 2009; Dudhia, 2017). Here we use the profiles generated by the Institute of Meteorology and Climate Research (IMK) in cooperation with the Instituto de Astrofísica de Andalucía (von Clarmann et al., 2009) in particular version 5. MIPAS IMK/IAA algorithm retrieves temperature and more than 30 species including O_3, H_2O, CO, CFCs, PAN, among many others. This retrieval algorithm uses a Tikhonov regularization; it is capable of handling deviations from local thermodynamic equilibrium, and it includes temperature horizontal gradients along the line of sight to prevent many retrievals from failing to converge, particularly near the boundary of the poles. Horizontal gradients are important because the line of sight extends around a thousand kilometers, crossing situations where the assumption of horizontal homogeneity is unrealistic (i.e., 1D retrievals). Several studies have discussed the advantages of including inhomogeneities along the line of sight for atmospheric retrievals (e.g., Livesey and Read, 2000; Carlotti et al., 2001, 2006; Kiefer et al., 2010; Castelli et al., 2016).

MLS (Waters et al., 2006) was launched in July 2004 on the Aura spacecraft. MLS measures limb millimetre and submillimetre atmospheric thermal emission in spectral regions near 118, 191, 240, and 640 GHz, and 2.5 THz. These radiances are inverted using a 2D tomographic optimal estimation algorithm (Livesey et al., 2006) that allows the retrieval of temperature and composition. MLS measures around 3500 vertical scans daily, providing near-global (82°S to 82°N) observations.

To investigate the impact of sampling and quality screening, daily CMAM30-SD model fields were linearly interpolated to the actual latitude and longitude of the satellite measurements. For the MIPAS sampling pattern, for each calendar day of the year we identify the year with the most measurements obtained on that date. That is to say, for the 1st of January, we use the locations of the 1st of January for the year with the most measurement locations, etc. This allows us to have a complete year of MIPAS measurements without interruptions due to MIPAS changing measurement modes. For MLS, we use 2008 as a representative year. To avoid differences attributed to diurnal cycles, all satellite measurements were assumed to be made at 12:00 UT on a given day, avoiding any interpolation in time. Further, we used the vertical grid of the CMAM30-SD fields; that is, the impact of the vertical resolution of the measurements is not taken into account. However, note that, in this case, both instruments have similar vertical resolutions in the upper troposphere / lower stratosphere (UTLS), varying overall from 3 to 4 km.

We constructed three time series: one using the raw CMAM30-SD fields; another using all the measurement locations available; and lastly one using only the measurement locations remaining after the quality screening recommended for each instrument was applied, in other words, after those points flagged as bad values in the actual data were eliminated. The screening procedure applied to MIPAS data is as follows: We neglect profile points where the diagonal element of the averaging kernel is less than 0.03 — to avoid retrievals influenced by the a priori — and discard points where the visibility flag was set to zero — which indicates that MIPAS has not seen the atmosphere at those particular altitudes. The screening procedure applied to MLS data follows the guidelines detailed by Livesey et al. (2017): We only use data within the specified pressure ranges; we neglect profile points for which the precision is negative (which indicates that the retrievals are influenced by the a priori); we avoid profiles for which the "Status" field is an odd number (which indicates operational abnormalities or problems with the retrievals); and we only use profiles for which the "Quality" and "Convergence" fields are within the specified thresholds. The "Quality" field describes the degree to which the measured radiances have been fitted by the retrieval algorithm and the "Convergence" field is a ratio of the fit achieved at the end of the retrieval process to the value predicted at the previous step.

Figure 1 shows typical daily MIPAS and MLS geolocations overlaid on top of a modeled water vapor map. Both instruments have dense coverage that, as noted by Toohey et al. (2013), is relatively uniform with latitude and time. Figure 1 also displays those geolocations for which the retrieved values are not recommended for scientific studies, that is, they are screened out by the quality criteria. As shown, these failed or in many cases skipped retrievals cluster in the tropics or near the poles. Overall, in the tropics, these missing retrievals are due to clouds. Near the poles, the retrieval failures are presumably due to temperature horizontal gradients and, in the case of MIPAS, also due to the presence of polar stratospheric clouds. The substantial difference between the number of failed/missing retrievals in the tropics for MIPAS and MLS is the main motivation for this study.

To quantify this further, Figure 2 displays the yield given by,

$$Y = \frac{N_{QS}}{N_A} \quad (1)$$

where N_A is the number of measurements available and N_{QS} is the number of measurements left after applying the quality screening criteria at each latitude and each pressure level. Again, MIPAS low yield values accumulate in the tropics and near the poles. Overall, MIPAS yields drop below 60% near the South Pole at pressures greater than $\sim$20 hPa and below 30% in the tropics at pressures greater than 100 hPa. In contrast, in general MLS yield values are better than 90%, although the measurements do not extend below the upper troposphere. The two exceptions are the yield values for H_2O near the South Pole, which drop below 90%, and HNO_3 near the equator, which drop to 60%. Note that MIPAS yield values drop below 10% well into the troposphere.

3 Induced Sampling and Quality Screening Biases

Following Millán et al. (2016), we evaluate the sampling biases as well as the quality screening biases associated with constructing monthly zonal means using the raw CMAM30-SD fields, Z_R, versus those using the satellite-sampled measurements, Z_A, or only those passing the quality screening criteria, Z_{QS}. The difference between Z_A or Z_{QS} and Z_R gives the sampling or the quality screening induced bias, respectively. For each instrument and for each month throughout one year, we computed these biases as a function of latitude and pressure. Note that the quality screening bias is the sampling bias plus the additional impact of screening out more locations and, hence, reducing the sampling frequency.

Figure 3 shows examples of the sampling and screening biases for June 2005. Percentage biases are shown for the trace gases to cope with their large vertical variability. MIPAS and MLS sampling biases are practically identical. For the trace gases, sampling biases are larger in the upper troposphere, where the variability is larger, while the temperature sampling biases are larger near the edges of the polar regions, where there are substantial temperature gradients. The impact of the MIPAS quality screening is evident in the tropics (in particular near 20°N), where the yield values are expected to be greatly affected (see Figure 2) by clouds. In this region, on top of the sampling biases, all parameters studied display an underestimation, for example, up to -50% for H_2O. Although this resembles the expected dry bias in clear-sky tropospheric infrared measurements (e.g., Sohn et al., 2006; Yue et al., 2013) — that is, the fact that infrared instruments cannot measure cloudy regions where H_2O is high, resulting in a dry bias — the biases shown here are due to a combination of two factors: (1) high H_2O values associated with deep convection (the screened-out locations might not necessarily be cloudy in the model fields however they are for the most part in the tropics, in regions of high H_2O values, see Figure 1 for an example) and (2) due to the reduced sampling frequencies. Note that this is also applicable to other parameters; that is, the quality screening biases shown here are not an indication of trace gas (or temperature) / deep convection relationships. In contrast to those of MIPAS, except for the reduced vertical ranges, MLS sampling biases are unaffected by data quality screening.

We note that the cloud screening procedure of the IMK/IAA algorithm is conservative with respect to those of other MIPAS processors (Spang et al., 2012). On the face of it, it appears that this causes an unnecessarily large sampling bias which could be avoided by using a less restrictive cloud screening threshold value. The purpose of a conservative cloud screening procedure is to guarantee that the measurements passing the cloud screening are indeed unaffected by any cloud signal in the spectra. Cloud signals can lead to systematic retrieval errors, which are correlated to the state of the atmosphere, hence, the sampling biases would merely be replaced by retrieval biases. This, we think, is worse, because then both the parent data and the zonal averages would be affected, while with a conservative screening only the averages are affected but not the parent data which survive the screening.

To summarize the potential sampling and quality screening biases, Figure 4 shows their root-mean-square (RMS) computed over one year's worth of data. Again, the MIPAS and MLS RMS sampling biases are almost identical: H_2O displays a bias of up to 30% at pressures greater than ~150 hPa; CO, O_3 and HNO_3 show biases (up to 30% for O_3 and HNO_3) near mid-latitudes (around 40°S and 40°N), where there are sharp trace gas gradients and variability due to tropopause folding; and temperature displays a bias as large as 3 K near the polar edges.

The impact of MIPAS quality screening is especially evident in H_2O and HNO_3, which have potential biases as large as 100%, but quality screening also affects the rest of the parameters: CO and O_3 biases approach 30% in the tropics, while the region with 3 K temperature bias expands near the South Pole. As before, except for the reduced vertical ranges, the impact of the MLS quality screening is negligible; that is, the screening biases are almost identical to the sampling biases.

To exemplify the impact of these quality screening biases, Figure 5 (left) shows time series (1979-2012) of 20°S to 20°N H_2O at 200 hPa using the raw CMAM30-SD fields, the full satellite-sampled fields and only those points passing the screening criteria. All time series show the expected features, with an annual cycle related to the seasonality of the cold point tropopause temperature. The MIPAS time series constructed using the full satellite-sampled fields is almost identical to the one constructed using the raw CMAM30-SD field. However, as suggested by the screening bias shown in Figure 4, the MIPAS time series using the quality screening displays a substantial dry bias. In contrast, no evidence of such a bias is seen in the MLS time series; that is, both the time series constructed using the full satellite-sampled field and that based on only those points passing the screening criteria are almost identical to the CMAM30-SD one.

Figure 5 (right) shows the area-weighted scatter between these time series. MIPAS sampling scatter, that is, the scatter between MIPAS when using all available measurements and the raw CMAM30-SD fields, is small and their correlation tight, with a bias better than -1.5%, a slope of $\sim$1.05, and a coefficient of determination of 0.98. The contrast with the MIPAS screened scatter is dramatic in this particular latitude/pressure region; it displays considerably more scatter and, as in the time series (Figure 5-left), a discernible bias. Quantitatively, MIPAS screened data displays a bias of 16.13%, a slope of 1.32, and a coefficient of determination of $\sim$0.8 (which implies that 20% of the total variation cannot be explained). MLS sampling and screened scatterplots are almost the same.

To explore this further, Figure 6 shows these metrics versus pressure using different latitude bands for the MIPAS sampling scatter. As shown, the coefficients of determination as well as the slopes are close to one and the biases close to zero in most cases. The most notable exceptions are the biases between 20° and 45° (either north or south) for O_3 and HNO_3, which can be up to -10%. In these regions, Figure 3 and Figure 4 indicate biases due to the sharp trace gas gradients associated with tropopause folding. Note that both the MLS sampling and the MLS screened scatter are almost identical to the MIPAS sampling scatter and, hence, are not shown.

The MIPAS screened scatter results are shown in Figure 7. The largest impact can be found in the tropics (the 20°S-20°N latitude band) at pressures greater than 100 hPa. Here, the coefficients of determination, the biases and the slopes are severely degraded. The coefficients of determination rapidly decrease, especially for H_2O, O_3 and HNO_3, whose values are as low as 0.5 at 200 hPa and worsen further at lower altitudes. The biases for O_3 and HNO_3 oscillate between -10% and 10% and can be as large as 40% for H_2O. Lastly, all the slopes vary from 0.5 to 1.5, depending on pressure level. These poor metrics imply that any trends derived at these pressure levels will also be impacted by quality screening induced biases: the magnitude of the trends will be affected because of the change in the slope, and the number of years of observations required to conclusively detect trends will considerably increase due to the noise associated with the worsening of the coefficients of determination (e.g., Millán et al., 2016). As an example, Figure 8 shows the H_2O and O_3 trends in the tropics computed using monthly zonal mean deseasonalized anomalies of the raw model fields, as well as using all the available satellite-sampled measurement locations and only those passing the screening criteria in the tropics. As shown, when all available measurement locations are used, the MIPAS and MLS sampling allows accurate derivation of trends, with values matching those calculated from the raw model fields almost exactly. However, when only those measurements passing the screening criteria are used, both instruments have limitations: MIPAS trends are impacted because of the large percentage of measurements screened out below 100 hPa, which introduces non-negligible artifacts (up to 80% change for H_2O and up to 20% change for O_3); MLS trends are impacted because of the reduced vertical resolution, which limits its usefulness to the upper troposphere and above. Note that the impact of quality screening on MIPAS trends can be mitigated by using a regression model similar to the ones used by Bodeker et al. (2013) and Damadeo et al. (2014). These models have been shown to mitigate the effects of the non-uniform temporal, spatial and diurnal sampling of solar occultation satellite measurements. Furthermore, MIPAS trend analysis can be restricted to regions less affected by deep convection (for example, the mid tropical Pacific) to minimize the quality screening effects.

The estimated number of years required to definitively detect these trends is also shown in Figure 8. These estimates were computed assuming a trend model similar to the one described by Tiao et al. (1990), Weatherhead et al. (1998), and Millán et al. (2016), with a seasonal mean component represented by the monthly climatological means. As shown, with the MIPAS screened fields additional years are required for robust trend detection (up to ∼150 years for H_2O and up to ∼40 years for O_3 versus 50 years and 20 years, respectively, when all available measurements are used).

Similar analyses were performed for other latitude bands. Although the magnitude of the trends derived when using the MIPAS screened measurement locations was also impacted in these cases, no significant difference was found in the number of years required to detect such trends. In addition, no significant artifacts were found for HNO3, CO or temperature for either the trend magnitude or the number of years required to detect such trends. Note that, when using real data, the effect of instrument noise upon trends will be negligible due to the vast number of MIPAS or MLS measurements associated with each monthly latitude bin. Drifts and long-term stability issues on these datasets (i.e., Eckert et al., 2014; Hubert et al., 2016; Hurst et al., 2016) will have to be corrected.

4 Summary and Conclusions

This study explored the implications of sampling in the UTLS for two satellite instruments, MIPAS and MLS, for H_2O, O_3, CO, HNO_3, and temperature. We quantify sampling biases by interpolating CMAM30-SD fields, used as a proxy for the atmospheric state, to the measurement locations and computing monthly means. Both of these instruments have dense uniform sampling, with around 1350 points spread globally for MIPAS and around 3500 spread from 82°S to 82°N for MLS, resulting in almost identical sampling biases for the two instruments. For the trace gases, the largest sampling biases are found in the upper troposphere, where there is more natural variability: H_2O displays a bias of up to 30%, while CO, O_3 and HNO_3 show biases near mid-latitudes of up to 10% for CO or 30% for O_3 and HNO_3 due to sharp trace gas gradients and variability arising from tropopause folding. The temperature sampling bias is negligible (less than 1 K), except near the polar edges, where the bias can be as large as 3 K, presumably due to horizontal temperature gradients.

Besides the orbital sampling biases, this study also evaluated the impact of quality screening, which further reduces the sampling frequency. In the tropics (see Figure 2), MIPAS is substantially impacted by clouds, as they act as grey bodies with high opacity, greatly altering the radiances below the cloud top. Cloud effects are evident, with H_2O and HNO_3 biases up to 100% and CO and O_3 biases up to 30%. In contrast, because of their longer wavelengths, MLS measurements are unaffected by all but the thickest clouds, negligibly impacting the sampling frequency. However, continuum absorption in the microwave suppresses signals from the mid and lower troposphere in a limb viewing geometry, limiting the MLS vertical range to the upper troposphere and above while MIPAS may cover well into the mid troposphere in cloud free scenes.

Analysis of scatterplots of time series constructed using the raw model fields versus those using all the available measurement locations (either for MIPAS or MLS) reveal that at most pressure levels and most latitude bands, the coefficient of determination and the slope of the fits are close to one, while the biases are close to zero. However, when only those measurements passing the screening criteria are used, MIPAS upper tropospheric measurements are severely impacted in some regions. In the tropics, the coefficients of determination rapidly decrease, especially for H_2O, O_3 and HNO_3, from $\sim$1 at 100 hPa to as low as 0.5 at 200 hPa, and they worsen further at lower altitudes. The biases for O_3 and HNO_3 oscillate between -10% and 10% and can be as large as 40% for H_2O. Lastly, all the slopes vary from 0.5 to 1.5, depending on pressure level. These biases affect trends derived from these measurements using a simple regression upon monthly zonal mean data substantially affected by clouds. Further, the number of years required to detect such trends may increase due to the extra noise added to the time series by screening out measurements. Note that although these results were derived for MIPAS, they are applicable to other instruments with dense sampling but for which quality screening (e.g., for clouds) severely impacts their yield.

5 Data availability

The datasets used in this study are publicly available: CMAM30-SD fields can be found in the Canadian Centre for Climate Modeling and Analysis webpage (http://www.cccma.ec.gc.ca/data/cmam/output/CMAM/CMAM30-SD/index.shtml), MLS data can be found in the NASA Goddard Space Flight Center Earth Sciences Data and Information Services Center (http://disc.sci.gsfc.nasa.gov/Aura/data-holdings/MLS/index.shtml), and MIPAS data can be found in the Karlsruhe Institute of Technology webpage (https://www.imk-asf.kit.edu/english/308.php).

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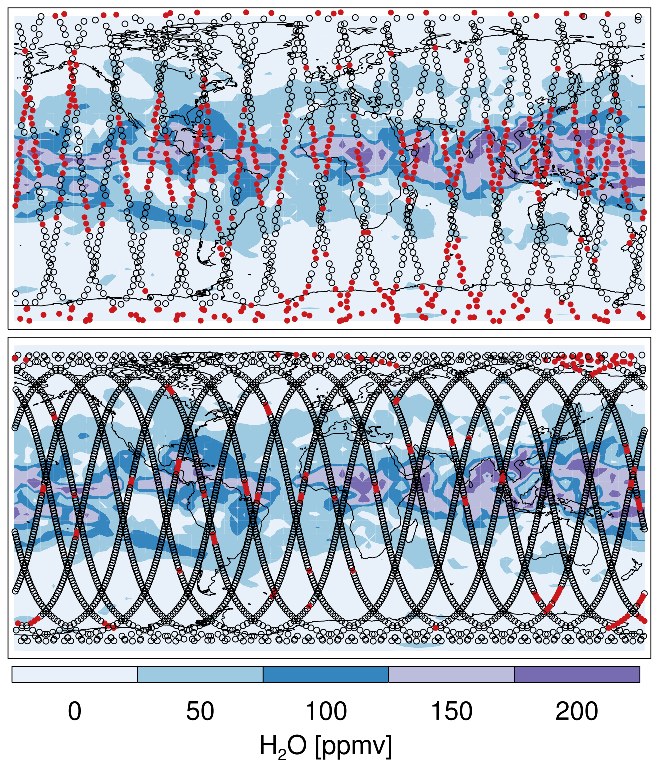

Figure 1. Typical MIPAS (top) and MLS (bottom) sampling overlaid on top of a modeled water vapor map (June 1st, 2005) at 200 hPa. Red dots show missed or failed retrievals: in the tropics, these are mostly due to clouds.

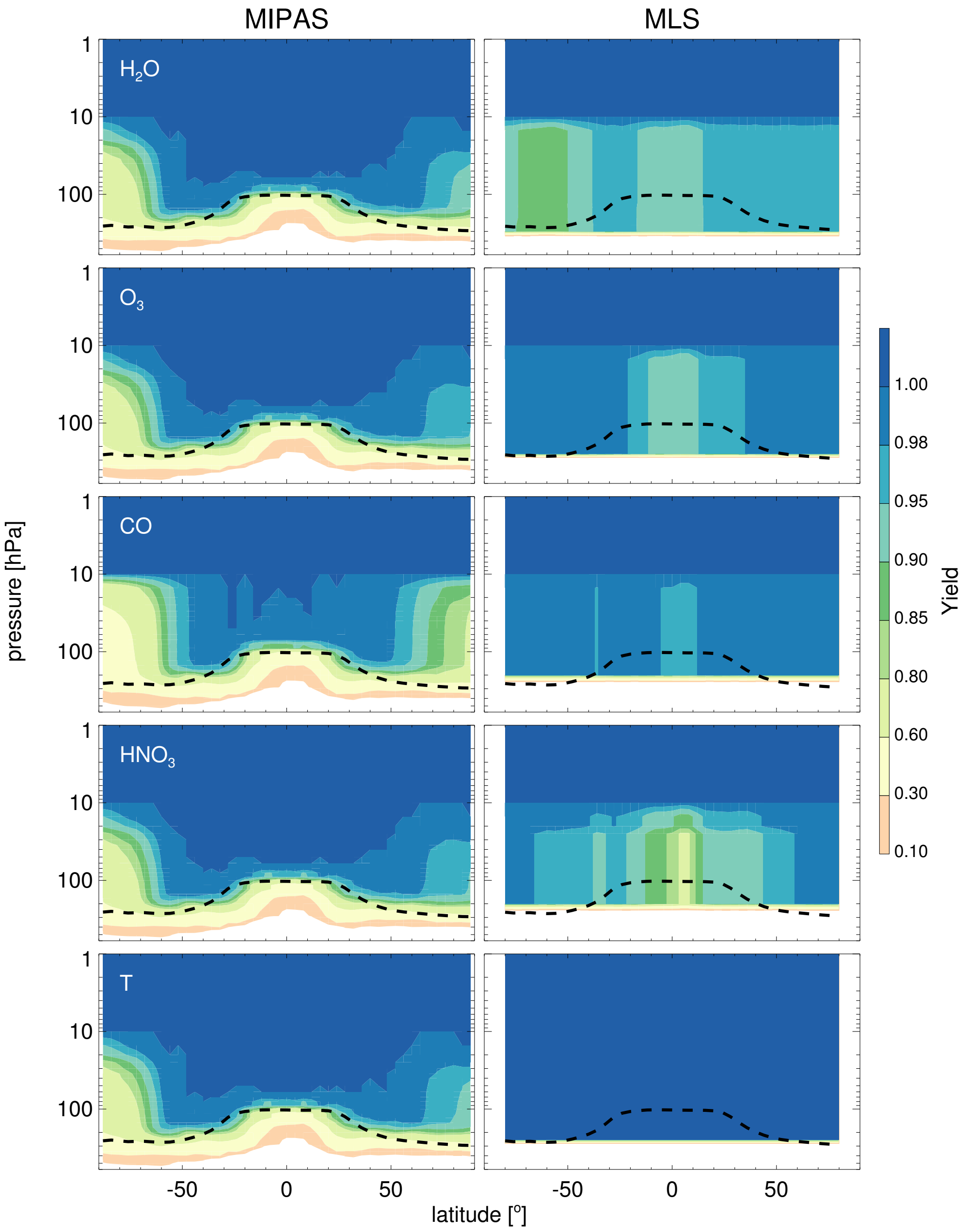

Figure 2. MIPAS and MLS zonal mean yield (N_{QS}/N_A where N_A is the number of measurements available and N_{QS} is the number of measurements left after applying the quality screening criteria) for H_2O, O_3, CO, HNO_3 and temperature for 2005, that is, sampling the modeled 2005 year with the sampling patterns as explained in the text. Note the non-linear color scale. The dashed black lines show the mean 2005 thermal tropopause derived from the Modern Era Retrospective Analysis for Research and Application-2 (MERRA2) fields (Bosilovich et al., 2015). This tropopause information was obtained from the derived meteorological products as described by Manney et al. (2007, 2011).

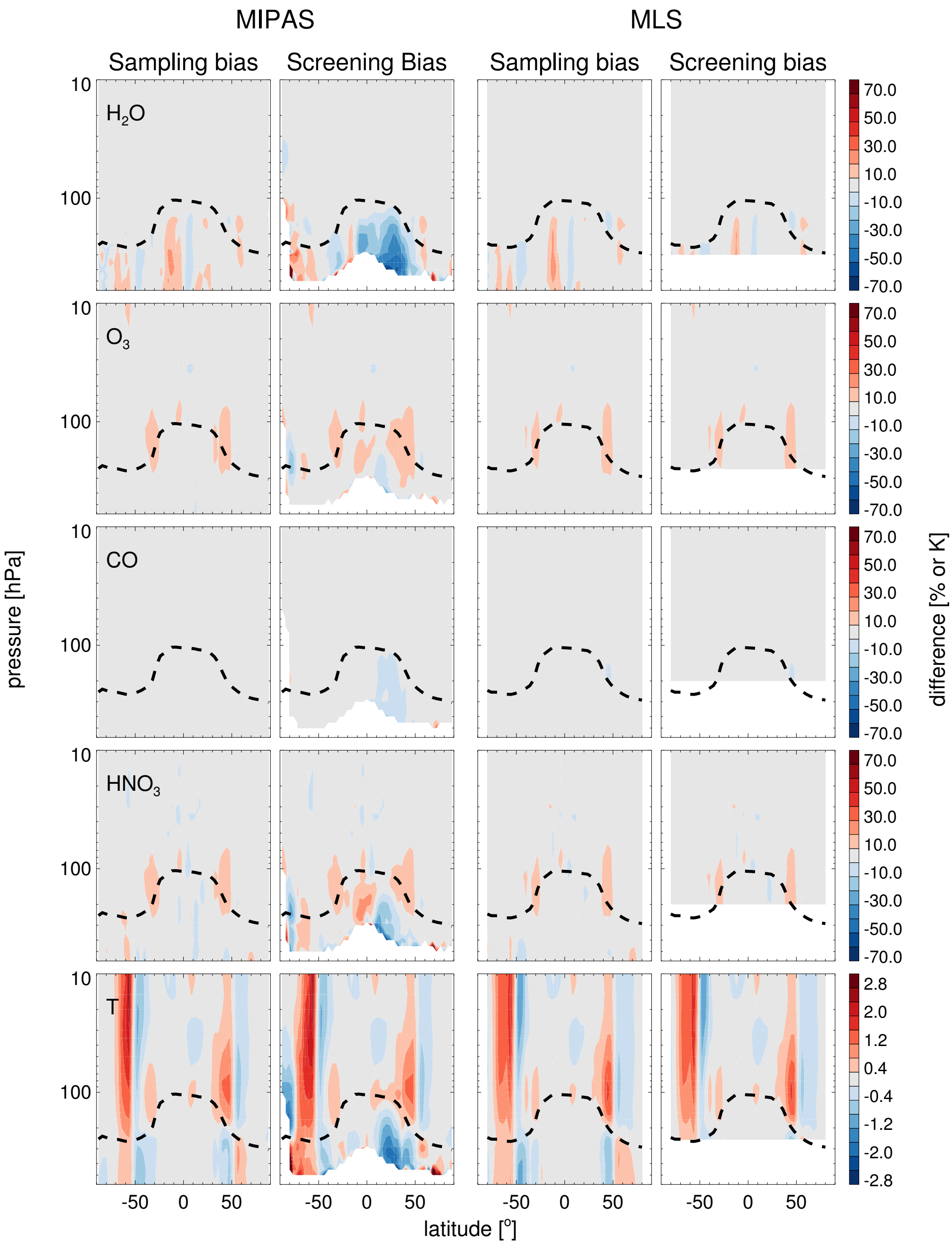

Figure 3. June 2005 sampling and quality screening biases as a function of latitude and pressure for H_2O, O_3, CO, HNO_3, and temperature as measured using MIPAS and MLS. White regions denote a lack of measurements. The dashed black lines show the mean 2005 thermal tropopause derived from MERRA2.

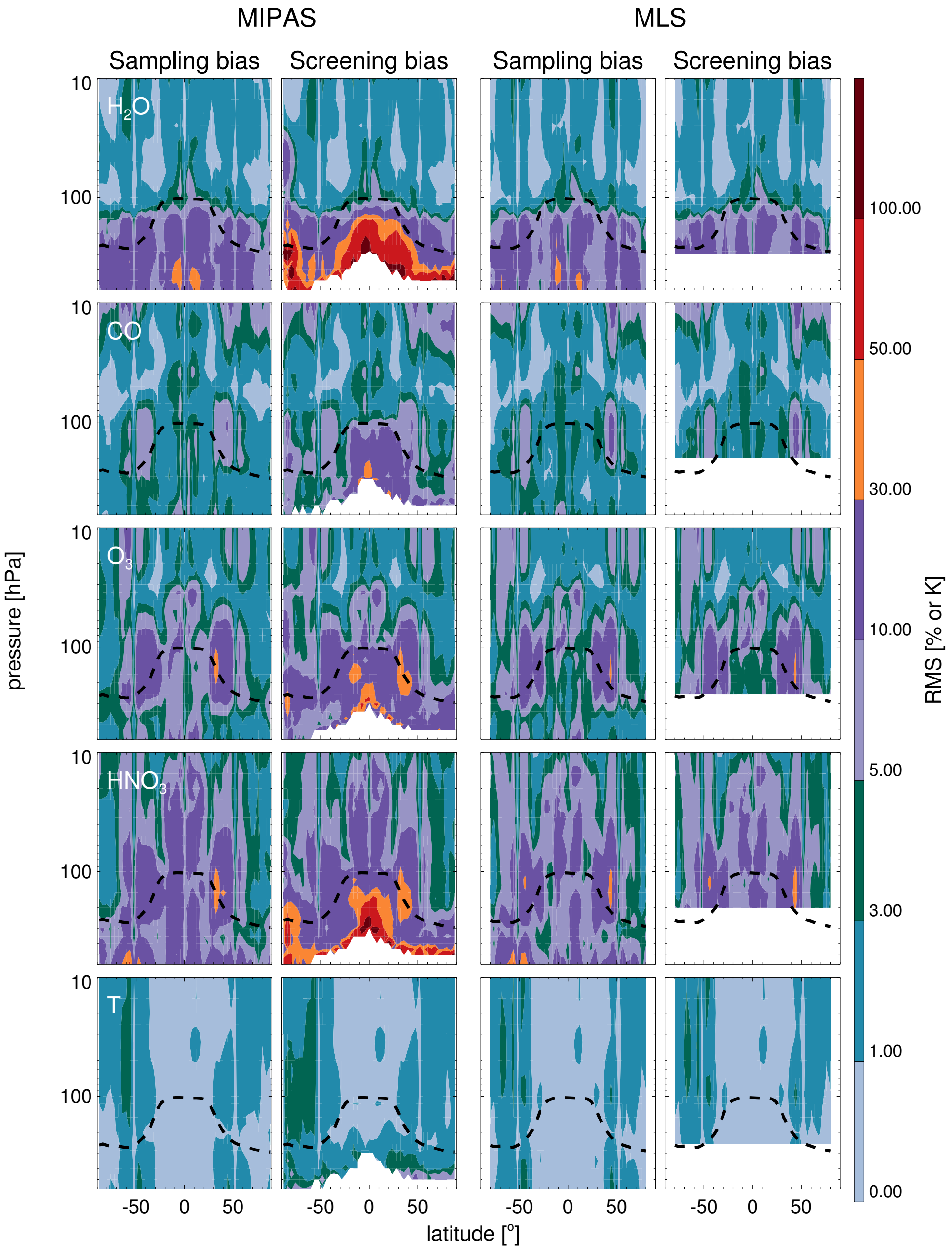

Figure 4. Root-mean-square sampling and quality screening biases for 2005 as a function of latitude and pressure for H_2O, O_3, CO, HNO_3, and temperature as measured using typical MIPAS and MLS data coverage. The dashed black lines show the mean 2005 thermal tropopause derived from MERRA2.

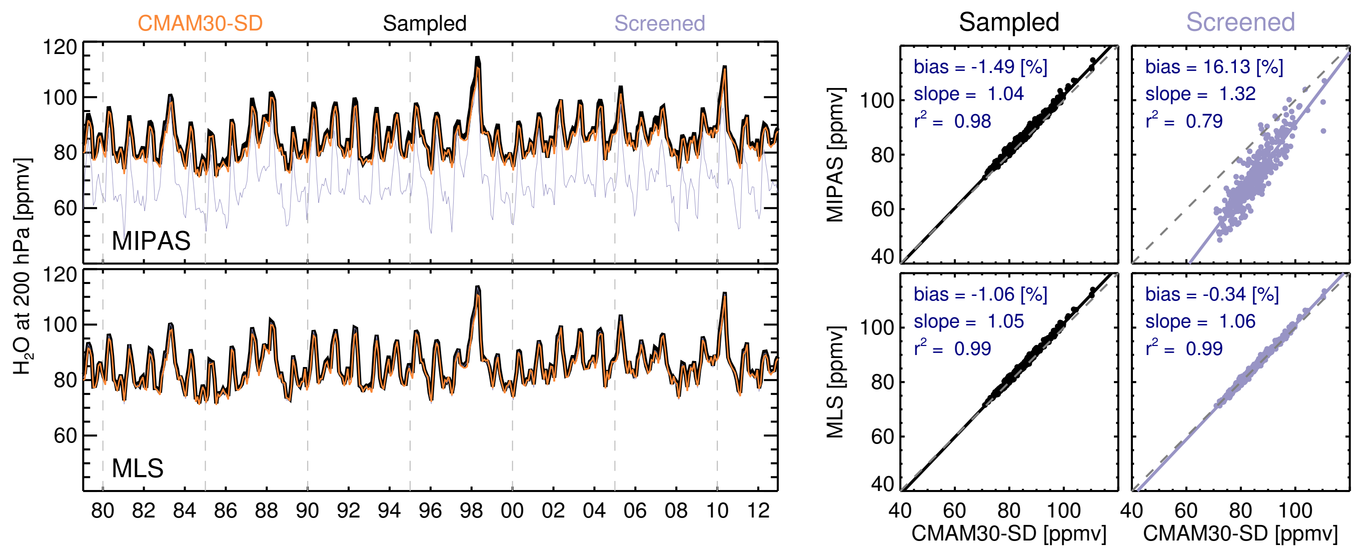

Figure 5. (left) Time series of 20°S-20°N H_2O at 200 hPa for the raw CMAM30-SD fields (orange lines), the full satellited-sampled fields (black lines) and only those points passing the quality screening criteria (thin purple lines) for MIPAS and MLS. (right) Scatterplots between these time series. The dashed gray lines are the 1:1 line, and the solid lines are the linear best fits, whose slopes are given. Also, the coefficient of determination, r^2, and the bias are shown.

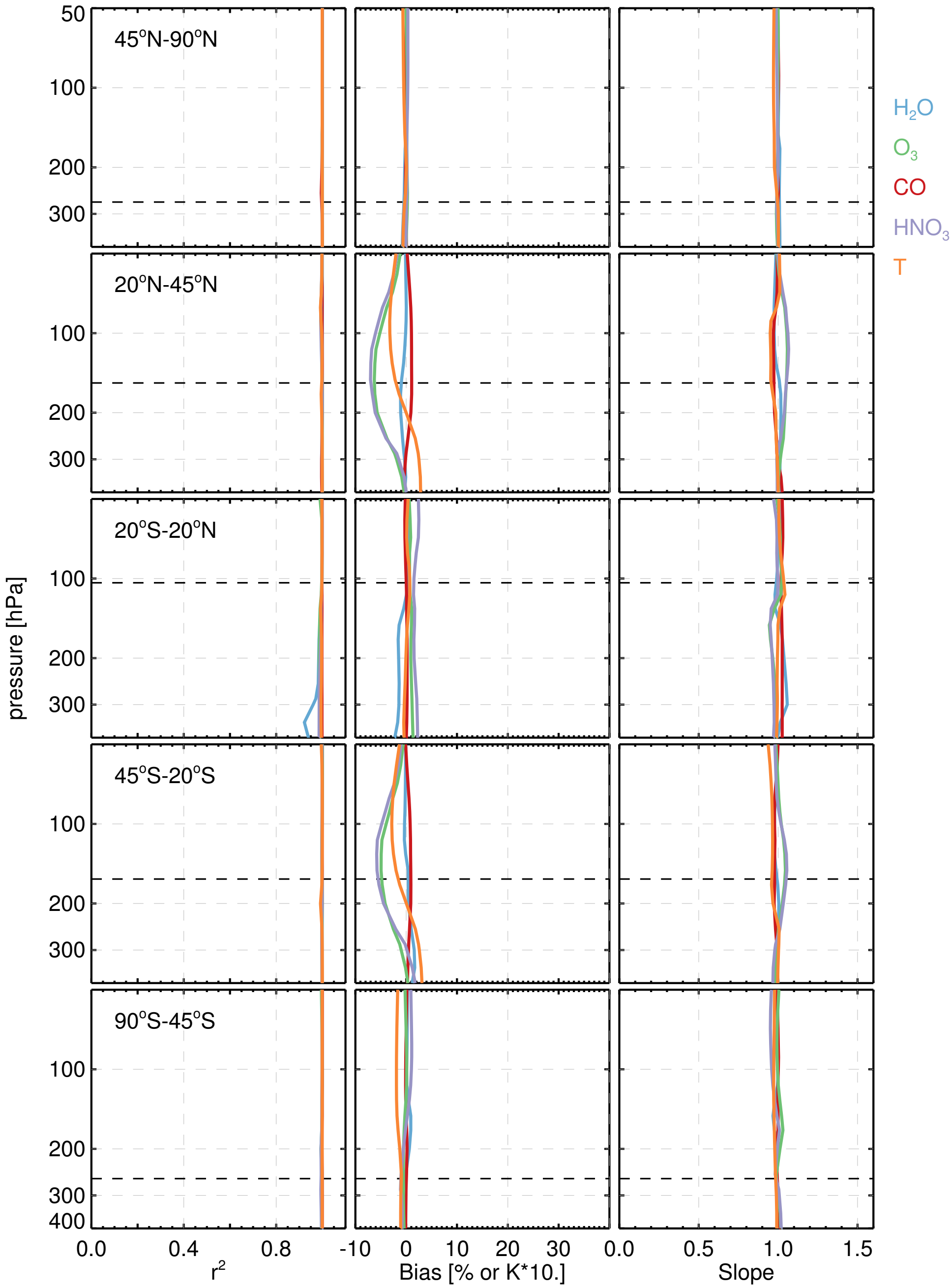

Figure 6. Vertical profiles of the coefficient of determination, the bias, and the linear fit slope for different latitude bands for the MIPAS vs CMAM30-SD scatter using the full satellite-sampled fields. Note that for clarity the temperature bias is shown as K*10. Blue, green, red, purple, and orange lines represent H_2O, O_3, CO, HNO_3, and temperature metrics. The dashed black lines show the mean 2005 thermal tropopause derived from MERRA2 for the particular latitude bands.

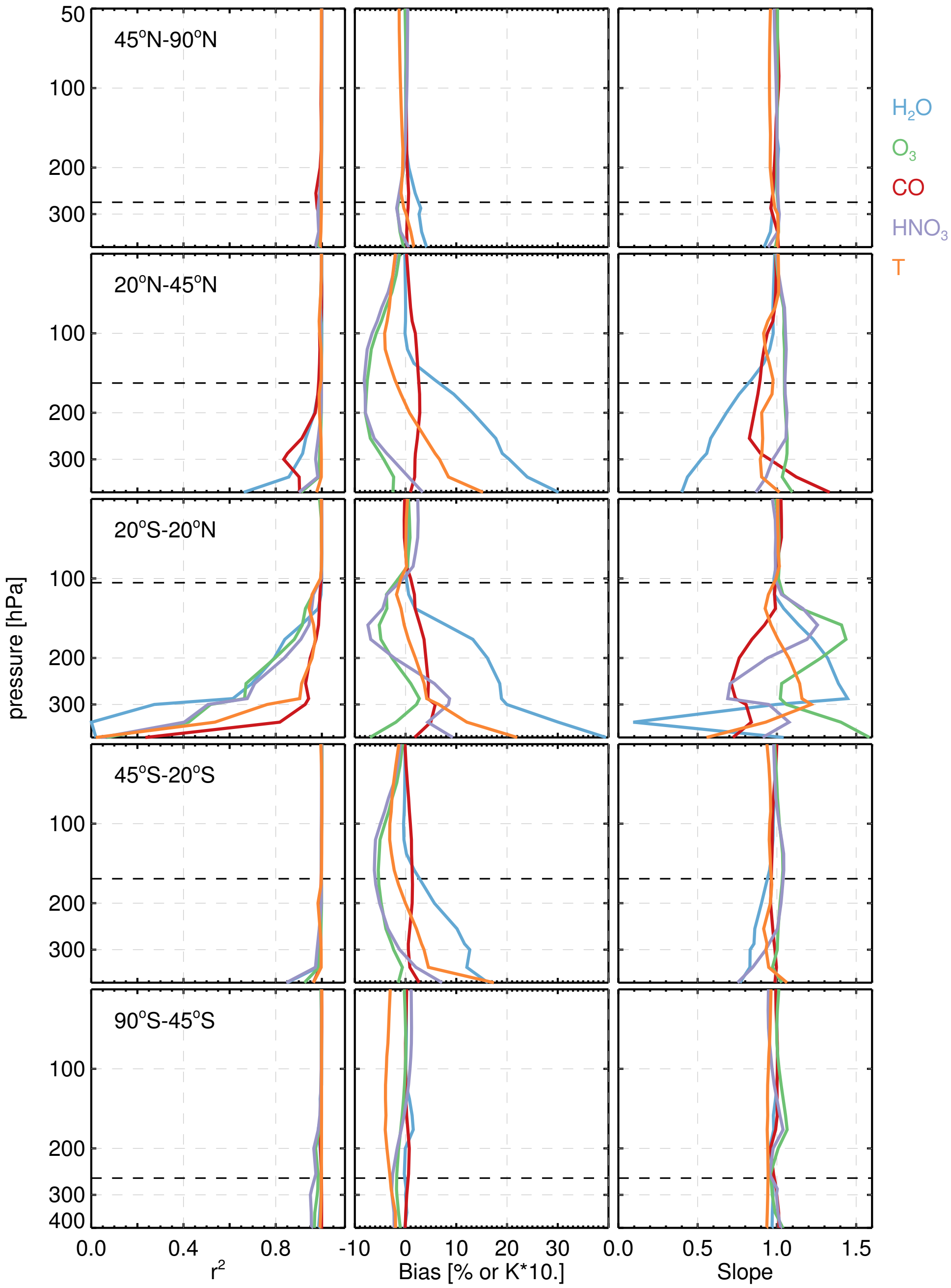

Figure 7. As in Figure 6 but using only the profiles that passed the quality screening.

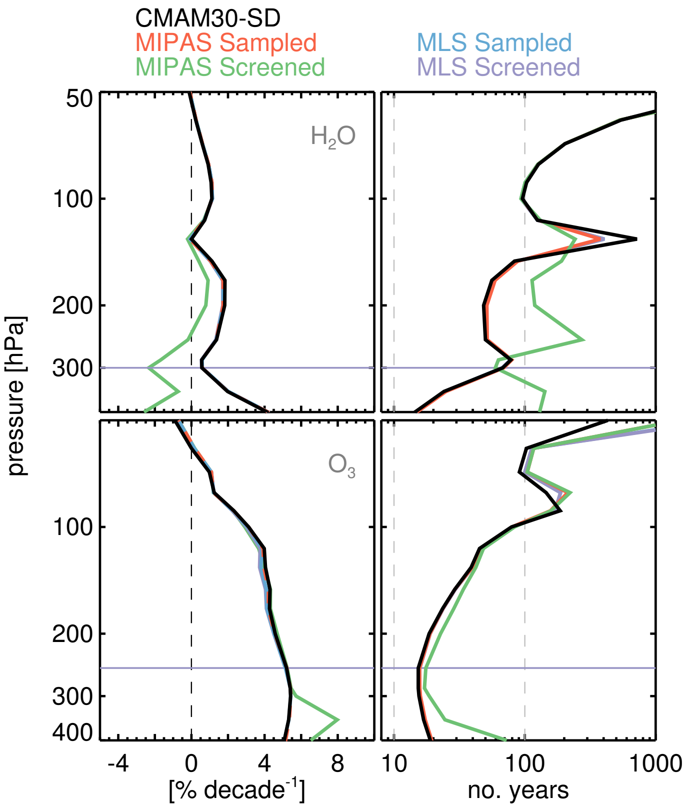

Figure 8. (left) H_2O and O_3 trends computed based on monthly zonal mean deseasonalized anomalies for the tropics (20°S to 20°N) using the raw model fields, all the available satellite measurements (MIPAS or MLS sampled) and only those measurements passing the screening criteria (MIPAS or MLS screened). Note that for O_3, we only use data starting from 2000 to capture the expected period of O_3 recovery. A purple line indicates the bottom (largest pressure) of the recommended range of the MLS retrievals. (right) Number of years required to detect such trends.