Response to RC1:

Thank you for your thorough review and thoughtful comments on our manuscript. We agree that we did not adequately explain the significance of our validation results for monitoring Earth system change. We have revised the manuscript to address this important concern. Our responses to each of your comments and questions are listed below in italic font.

RC1: <u>'Comment on amt-2021-211'</u>, Anonymous Referee #1, 23 Aug 2021 <u>reply</u> The authors present an in-depth error analysis of the AIRS MUSES CO retrieval product. The MUSES algorithm follows the Rodgers optimal estimation approach (OE), which allows them to quantify a smoothing error, measurement noise, systematic uncertainty, cross-state error and retrieval residual. They use these to derive four error terms – theoretical, a-priori, retrieval, and empirical – for MUSES CO retrievals collocated with aircraft observations made during the HIPPO, ATom and NOAA GML campaigns. For each campaign, the authors repeat their analysis and present four figures and a table.

This paper summarizes an extraordinary amount of meticulous work about an important topic in satellite retrieval theory and application today, namely error quantification and validation. The authors acknowledge the importance of understanding all the retrieval error terms if we are to use a satellite record in climate science and the quantification of Earth system change. This is especially true for the AIRS record that now spans two decades. But as this paper makes clear, this is no easy task. I have spent some time with this paper, revisiting sections, and am left with the conclusion that while the authors present clear, detailed results, they fail to communicate what it all means. It would have been very helpful to the reader if the authors explained how these results will be used to improve the MUSES algorithm (or product) going forward, or what this error evaluation means for the AIRS record and its application in Earth system science. After working through all the details, trying to understand the results, I (the reader) am left thinking "so what?". This paper can make a meaningful, even important, contribution if the authors elaborate on the significance of their results in the Discussion/Conclusion.

This validation study and the results presented in this paper are significant for the following reasons.

1. We validate AIRS single footprint retrievals which can better resolve smaller pollution plumes, such as those generated by small-scale fires than the operational AIRS product that is produced from the 3 x3 array of AIRS footprints. For example, the plot below shows single footprint AIRS CO retrievals from the WE-CAN campaign as colored circles with the bounding box of the 3 x 3 array field of regard overlaid. The shape of the CO plumes and the higher values from the fires are well represented but would be smoothed out in the lower-resolution AIRS operational product. While this figure is not part of our study and not included in the paper it illustrates visually the impact of finer spatialresolution.



To better emphasize the importance of the higher resolution we added the following sentences to the Introduction starting on line 89 of the original manuscript.

"The improved spatial resolution enables better representation of smaller pollution plumes from local strong anthropogenic sources and small wildfires which will enable better pollution tracking and more precise trend analysis. For example, George et al (2009) found that CO related to fires was systematically ~ 17 % lower for AIRS than MOPITT and IASI due to AIRS's coarser resolution. Furthermore, Buchholz et al (2021) using MOPIIT found that recent trends in column CO over northeastern China were driven mainly by significant trends in the 75th percentile values suggesting changes in local rather than regional emission sources."

2. The validation of the observation error (as reported in the satellite products), spatial variation in bias and any time drift in the bias are important for use of this AIRS CO data in emissions estimation and/or chemical reanalysis. Our results do not show an appreciable latitudinal dependence in the bias. Furthermore, our results show that the bias drift over time is small (~0.5%).

3. Our results suggest that the reported /estimated observation errors are low by a factor of up to ~2. In Figure 5 (particularly in the 30N – 60N band) and Figure 13 the AIRS- Aircraft standard deviations are much larger than the reported observation errors. This indicates that observation errors are an underestimate of the actual retrieval error. The cause is not yet determined but is being investigated.

We have made substantial revisions to the Discussions and Conclusions section to better emphasize points 1-3 above.

Review:

 Lines 37-39: "We find mean biases of + 6.6% +/- 4.6%, +0.6% +/- 3.2%, -6.1% +/-3.0%, and 1.4% +/- 3.6%, for 750 hPa, 510 hPa, 287 hPa, and the column averages, respectively. The mean standard deviation is 15%, 11%, 12%, and 9% at these same pressure". This sentence is very difficult to read and I suggest rephrasing it to help clarify one of the main results of this paper.

These sentences have been changed to the following. "We found mean biases of + 6.6% +/- 4.6%, +0.6% +/- 3.2%, and -6.1% +/- 3.0% for three representative pressure levels of 750 hPa, 510 hPa, 287 hPa, and column average mean biases of 1.4% +/- 3.6%. The mean standard deviations for the three representative pressure levels were 15%, 11% and 12% and the column average standard deviation was 9%."

• Line 143: "Atmospheric Infrared Sounder (AIRS)" already defined

Changed "The Atmospheric Infrared Sounder (AIRS) is" to "AIRS is".

• Line 164: "CO is retrieved using the 2181-2200 cm-1 spectral range". Does MUSES use all channels in this spectral range for its CO retrieval?

Yes, this is correct.

• What does MUSES use as a-priori for CO? I think it is important to state this clearly in the paper given the results presented later.

The a priori profiles for CO are derived from from a monthly climatology, in 30 degree latitude by 60 deg longitude boxes and there is no variation in this climatology from one year to the next. The climatology was produced from MOZART model output, from runs performed for construction of climatologies for the Aura mission [Brasseur et al., 1998]. The a priori constraint used for CO is the same constraint used in the MOPITT CO algorithm [Deeter et al., 2010].

the MOZART model. We have added the following to Line 225 of the original manuscript.

"For AIRS MUSES CO retrievals, the a priori profiles are obtained from a monthly climatology, in 30 degree latitude by 60 deg longitude boxes produced from the MOZART atmosphere chemistry model for the Aura mission (Brasseur et al., 1998). The a priori constraint used for CO is the same constraint used in the MOPITT CO algorithm [Deeter et al., 2010]."

"Brasseur, G. P., Hauglustaine, D. A., Walters, S., Rasch, P. J., Muller, J. F., Granier, C., and Tie, X. X.: MOZART, a global chemical transport model for ozone and related chemical tracers 1. Model description, J. Geophys. Res.-Atmos., 103, 28265–28289, 1998." Deeter, M. N., et al. (2010), The MOPITT version 4 CO product: Algorithm enhancements, validation, and long-term stability, J. Geophys. Res., 115, D07306, doi: <u>10.1029/2009JD013005</u>

We have also added the citations above to the References section.

MUSES does not follow the AIRS Science Team approach of deriving an aggregate clear-sky radiance from each 3 x 3 array of AIRS measurements in partly cloudy skies. While cloud clearing reduces the spatial resolution of the radiance measurements ahead of retrieval, it not only allows stable retrievals in complex scenes but also allows the quantification of uncertainty due to clouds (Smith and Barnet, 2019; Susskind et al., 2014; Maddy et al., 2009; Chahine, 1982, 1977). Clouds being one of the primary sources of scene-dependent uncertainty, this is an important source to account for in an error analysis. How does MUSES quantify systematic uncertainty due to clouds? And given the results presented, can the authors draw any conclusions about the validity of retrieving CO from AIRS measurements in the presence of clouds?

MUSES retrieves cloud optical depth following Kulawik et al (2006). The retrieval provides both spectrally dependent and full spectrum average effective cloud OD and an effective OD. In our analysis the effective cloud optical depths to remove retrievals using a threshold effective cloud optical depth of 0.1. We have added the following text starting on Line 178 of the original manuscript.

"While the AIRS MUSES algorithm uses the original single pixel instrument radiances rather than cloud-cleared radiances, the algorithm does retrieve cloud optical thickness following Kulawik et al (2006) and provides both a spectrally varying and average effective optical depth. The cloud optical depth is retrieved before CO, thus the effect of clouds is taken into account in the CO retrieval. AIRS MUSES profiles with optically thick clouds were designated as those with an average cloud effective optical depth over the AIRS spectrum and within the CO absorption band greater than 0.1 and were removed from the set."

We have also added to the Reference section the following citation.

"Kulawik, S. S., Worden, J., Eldering, A., Bowman, K., Gunson, M., Osterman, G. B., Zhang, L., Clough, S. A., Shephard, M. W., and Beer, R.: Implementation of cloud retrievals for Tropospheric Emission Spectrometer (TES) atmospheric retrievals: part 1. Description and characterization of errors on trace gas retrievals, J. Geophys. Res.-Atmos., 111, D24204, https://doi.org/10.1029/2005JD006733, 2006."

• Line 175: "the original non cloud-cleared radiances". It will be more straightforward to simply say "the instrument radiances"

We think it is important to emphasize here that the radiances used have not been subjected to cloud clearing and therefore could be affected by the presence of optically thick clouds. That sentence has been changed to read "Since the AIRS MUSES algorithm uses the original instrument radiances rather than cloud-cleared radiances, profiles with optically thick clouds diagnosed by the AIRS MUSES algorithm were also removed from the set."

• Line 178: "profiles with thick clouds were also removed from the set." How did the authors distinguish thick (versus thin) clouds?

Thick clouds would be those with an effective cloud optical depth greater than 0.1. To make this point clearer the sentence starting on Line 178 has be rewritten as "AIRS MUSES profiles with optically thick clouds were designated as those with an average cloud effective optical depth over the AIRS spectrum and within the CO absorption band greater than 0.1."

• Figure 2 needs to be resized.

We can resize it (make it smaller) in the final draft.

• It is difficult to make sense of the results in Tables 1 through 3. I think a single figure summarizing the values from all three would have made it easier to inter-compare among latitude zones and aircraft campaigns.

Table 4 shows average or summary statistics for all campaigns. We have also added three rows for the overall statistics for each of the three campaigns to this table to facilitate inter-campaign comaprisons.

• Lines 285-286: "Beyond examining biases and variability of the retrieved profiles, evaluating the retrieval error estimates is also important, since they provide users with a measure of the reliability of the data". I agree with this statement in principal but "provid[ing] users with a measure of the reliability of the data" is what bias and standard deviation tells the user at first order. What, in the authors experience, do an error analysis contribute over and above a measure of reliability? Perhaps the authors can clarify this point with examples on how such an error analysis influences algorithm design/updates and data application.

As stated in our response to the general comments our results suggest that the estimated observation errors are low by a factor of up to ~2, particularly in the 30N – 60N band. Furthermore, the AIRS- Aircraft standard deviations are much larger than the reported observation errors. These findings indicate that observation errors are an underestimate of the actual retrieval error. The cause of this underestimate is still under investigation.

• Figures 5, 9, 13:

Is it correct to interpret this figure as meaning that the MUSES retrieval basically added noise to the a-priori between the Earth surface and 600 hPa?

No, this just indicates where the sensitivity is and is dependent upon natural variability in the retrieved scenes (e.g., T, Q, CO etc.) and large spatiotemporal coincidence criteria.

How sensitive are these error values to variation in a-priori error?

The observation errors shown in Figs 5, 9, 13 are not sensitive to variation in the a priori error covariance. The observation error is the sum of the covariances associated with noise and cross-state terms. The smoothing error term (which is impacted by the a priori covariance) is not included in the observation error.

What would be an ideal relationships between all these error terms?

Ideally you would be measuring exactly the same air mass and the computed observational error would match the standard deviation of AIRS – Aircraft. However, this is not feasible, since AIRS will always measure a larger volume vertically and horizontally than the aircraft, even if the latter is spiraling.

Do the authors think that the observation error in the lower troposphere will change if they adjust the a-priori error vertically?

It would change the profile retrieval and smoothing error but not observational error.

The legend states "mean observation error", "mean a priori error", 'AIRS-AIRCRAFT Std. Dev" and "A Priori-AIRCRAFT Std. Dev", but in the text associated with these figures, the authors discuss the "theoretical error" and "empirical error". It will help the reader a great deal if the authors maintain consistency in their terminology.

Please note that the references to "mean observation error", "mean a priori error", 'AIRS-AIRCRAFT Std. Dev" and "A Priori-AIRCRAFT Std. Dev" in the text are referring to Figures, 5, 9 and 13 while the terms "theoretical error" and "empirical error" refer to an alternative error analysis approach illustrated in Figures 6 and 10. However, it is correct that the "theoretical error" in Figures 6 and 10 is the calculated in the same way as the "mean observation error" but just for a set of AIRS profiles collocated with a single aircraft profile rather than an entire latitude band.

We have changed the legends in Figures 6 and 10 and the text referring to them to maintain consistency. The term "theoretical error" has been replaced with "mean observation error" (to be consistent with the terminology of Figures 5, 9 and 13) and the term "empirical error" has been replaced with "AIRS profile variability", which is a more descriptive name. Note that the "AIRS profile variability" was estimated as the square root of the diagonal of the covariance matrix of all the coincident AIRS MUSES retrievals with a particular aircraft location and is different from the AIRS – AIRCRAFT standard deviation which is a measure of the variability of the actual retrieval error.

We have also changed the introductory information related to the alternative approach related to Figures 6 and 10 on Lines 310 – 312 in the original manuscript to the following.

"An alternative approach for evaluating the theoretical error is to compare it to the variability within the set of AIRS profiles collocated with an aircraft profile. If it is assumed that all satellite footprints in the collocated set are basically seeing the same scene then the

variability in the retrieved profiles can be considered an empirical error (Oetjen et al., 2014). In this analysis this empirical error is referred to simply as the AIRS profile variability."

Do these results mean that an end user should use the a-priori instead of the retrieval in the lower troposphere?

The retrieval products include the averaging kernel for each retrieved profile. The averaging kernels are scene-dependent. For each profile, the averaging kernel provides information on how strongly the retrieved profile is influenced by the prior vs the measured radiances at any given altitude. The end user should use the retrieved profile together with the averaging kernel.

In general, the AIRS CO retrievals do not provide information on CO variations close to the surface, so if the end user is primarily interested in near-surface CO, they should be looking for a different product.

• Line 277/Line 355: Figure 3/Figure 7 captions, "The number of profiles and the latitude bands are indicated in the upper left". I only see the sampling size listed, not the latitude band.

We have added the latitude band information to these figures.

• Figure 11 should be resized.

We will resize this figure for the final draft.

• Line 603: "AIRS MUSES algorithm indicated that the retrieval quality was generally within expected limits." What are these limits?

We have changed this statement to read "Estimated theoretical observation errors from the AIRS MUSES algorithm were generally small as expected in the middle troposphere where AIRS has good sensitivity."

 Given this in-depth analysis of multiple error sources, what does it mean for AIRS product design? What are the lessons learned for algorithm teams and/or end user applications?

The important findings for the end users are that there doesn't appear to be a strong latitudinal dependence of bias and that the bias drift over time is small. This suggests that the data can be used to compare regional differences in CO mixing ratios and to track trends over time.

For the algorithm team the fact that the observation errors are underestimating the actual retrieval errors suggests that adjustments could be made to the constraints used in the algorithm.

References

Chahine, M. T.: Remote sounding of cloudy parameters.II. Multiple cloud formations, J. Atmos. Sci., 34, 744–757, 1977.

Chahine, M. T.: Remote sensing of cloud parameters, J. Atmos. Sci., 39, 159–170, 1982.

Maddy, E. S., Barnet, C. D., and Gambacorta, A.: A computationally efficient retrieval algorithm for hyperspectral sounders incorporating a-priori information, 6, 802–806, https://doi.org/10.1109/LGRS.2009.2025780, 2009.

Smith, N. and Barnet, C. D.: Uncertainty Characterization and Propagation in the Community Long-Term Infrared Microwave Combined Atmospheric Product System (CLIMCAPS), 11, 1227, https://doi.org/10.3390/rs11101227, 2019.

Susskind, J., Blaisdell, J. M., and Iredell, L.: Improved methodology for surface and atmospheric soundings, error estimates, and quality control procedures: the atmospheric infrared sounder science team version-6 retrieval algorithm, 8, 084994, https://doi.org/10.1117/1.JRS.8.084994, 2014.