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Atmospheric Measurement Techniques Discussions

Interactive comment on "Evaluation of single-footprint AIRS CH_4 Profile Retrieval Uncertainties Using Aircraft Profile Measurements" *by* Susan S. Kulawik et al.

Susan S. Kulawik et al.

susan.s.kulawik@nasa.gov

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Thank you to the reviewers for their helpful comments. The format of this response is alternating paragraphs of: reviewer comment, response, reviewer comment, response... The ordering of the responses are: major comments from reviewer 2 and minor comments from reviewer 2 (comments taken from the embedded PDF).

Reviewer 2 major comments:

Reviewer 2: (1) During first reading I got confused at several instances because an error was introduced by number, while the path towards derivation of this error was

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only explained in the next para or section. I always thought I have missed a part of the manuscript but found out with re-reading that the explanation follows on the number. It would be easier (at least for readers like me) to first provide the explanation and then the number.

Response: A reference to the section where each is calculated was added, or the "preview" was removed. "Figure 3 shows the predicted errors for the AIRS partial column XCH4 VMR within the pressure levels measured by the aircraft. The measurement error (light green) is 18 ppb (from the last term of Eq. 7b) , and the total error for a single observation (including smoothing error) is 41 ppb. A component of the total error, the cross-state error, is estimated as 21 ppb (from Eq. 7b)." The smoothing error estimate now shown after the new Eq. 5 and the text states that this is calculated from Eq. 5.

Reviewer 2: (2) The authors use very often the term "partial column". They need to introduce how the partial methane column over the pressure range the aircraft had measured has been calculated, both for the aircraft and AIRS data (what shape of the methane profile? where do pressure and temperature profiles come from?); further, the figures usually show volume mixing ratios (in ppb) instead of partial colums. This might sound picky, but I think this accurateness in wording should be kept.

Response: At the beginning of Section 2, 2 sentences were added to describe how partial columns are created, "The retrieval estimates AIRS CH4 dry volume mixing ratio (VMR) profile. When a "partial column quantity" is validated, the retrieved CH4 profile is post-processed into partial column XCH4 VMR relative to dry air, with methodology from Connor et al. (2008) and Kulawik et al. (2017), where the VMR's at the pressure levels are weighted according to a pressure weighting function, resulting in a partial column volume mixing ratio (VMR).". Based on reviewer 2's comments here and elsewhere, the paper was previously not clear that the partial column quantity is XCH4 VMR. The wording was updated throughout the paper to indicate that the validated quantity was "the AIRS partial column XCH4 VMR within the pressure levels measured by the aircraft"

Reviewer 2 (3): I was a bit surprised that the two models that were used to assess the so-called "validation error" (i.e. the unknown stratospheric part of the profile) provided largely different results (4.4 vs. 15.7 ppb). I think the authors should elaborate a little more on the reasons for this large difference. This is particularly important because the averaging kernels in Fig. 2 demonstrates that the stratospheric information is large mapped into the troposphere below 300 hPa, i.e. the AIRS signal obviously depends a lot on the assumptions about the stratosphere. Is it possible that the use of other models leads to even larger estimates of the validation error?

Response: Added additional text and reference on the errors from model extension of the aircraft profile: "The methane profile has a strong, spatially varying negative vertical gradient in the stratosphere. Models in general have a positive bias in the extratropical stratosphere (Patra et al., 2011). In GEOS-Chem 4x5, the column bias is shown in Figure 2c of Turner et al. (2015) and further discussed in Maasakkers (2019), which resolves the bias to the stratosphere, and model stratospheric accuracy is an active research area (Ostler et al., 2016; Maasakkers et al., 2019)."

Reviewer 2 (4) A side remark without relevance to the revision of this paper: the SPARC TUNER activity has worked on recommendations about error reporting. A paper on this topic has just been accepted by AMT. It would be nice to look into that paper (amt-2019-350) and possibly following these recommendations in future.

Response: Thank you for this information It is good to standardize validation.

Embedded notes/comments from Referee 2. I summarized the comments and wrote the response.

1) Abstract: Define "validation error" Response: Update wording in abstract, and also change name to "validation uncertainty" "We estimate a 16 ppb validation uncertainty because the aircraft typically did not measure methane at altitudes where the AIRS measurements have some sensitivity, e.g. the stratosphere, and there is uncertainty in the truth that we validate against."

Section 2: Question about how the partial column is defined and the profile shape assumptions. The text was updated in response to this and to an earlier comment to clarify that a profile is retrieved, and then an XCH4 VMR is calculated. "The retrieval estimates AIRS CH4 dry volume mixing ratio (VMR) profile. When a "partial column quantity" is validated, the retrieved CH4 profile is post-processed into partial column XCH4 VMR relative to dry air, with methodology from Connor et al. (2008) and Kulawik et al. (2017), where the VMR's at the pressure levels are weighted according to a pressure weighting function, resulting in a partial column volume mixing ratio (VMR)."

3) cm-1 formatting. Response: Updated.

4) removed URL from citation as suggested by reviewer.

5) Request figure 1: center legend on Pacific. Update symbols. Remove gray color. Label aircraft sites. Response: Updated as rerquested

6) Description of Sa is needed. Response: Updated section around the new Equation 5, "The expected total error includes the smoothing error, which the covariance of the hcAccxc-x ac (Rodgers, 2000), where the covariance of xc-x ac is the a priori covariance, Saxx. The smoothing error is: (Eq 5) We estimate the smoothing error for the partial column XCH4 VMR within the pressure levels measured by the aircraft to be 30 ppb, using Eq. 5. This estimate strongly depends on Saxx, the a priori covariance, which is the same as in Worden et al. (2012); briefly 5% diagonal variability with correlations in pressure set from the MOZART model."

7) Description of the selection of quality flags. "The specific flags used for AIRS CH4 are as follows, which were set by minimizing the standard deviation of small clusters of retrievals and to standardize the sensitivity:"

8) The reviewer suggests that things like "|KdotdL| < 0.23 should be given proper names. Response: Since these variables are not referred to outside of this section, and additionally are referencing an existing data user's guide, the updates were to the

description of the equation, e.g. |KdotdL| < 0.23 –> The absoluate value of KdotdL < 0.23.

Equation 1, question about "G" versus "Gr". Response: Removed the R. Thanks.

Question about "sum over i" in Equation 1. Response: change b to a vector and the summation is implied just like all the other matrix multiplication.

Comment on A = dx/dx "Careful with log! Response: Yes, thank you, the equations are mixing up x and log(x). The intention was that x=log(VMR), so A = dx/dx, and K = dradiance/dx = dradiance/d(log(VMR)). Other issues fixed in this section from the reviewer.

Reviewer: recomment on estimate of smoothing error. Response: Addressed above, the smoothing error was estimated from the new Eq. 5.

Reviewer at Eq. 5b, "It is necessary to mention that this step is possible because the levels of the aircraft measurement are assumed uncorrelated." Response: This is now Eq. 6a, and the text was updated, "Equation 6a accounts for all of the AIRS smoothing error, whereas Equation 6b (the equation used in this work, other than Section 3.3) only accounts for the smoothing error from the part of the atmosphere measured by the aircraft profile. [...] The difference from Eqs. 6a and 6b is discussed in Section 3.3. "

Eq 6, "This step comes as surprise. Including 1-2 steps or explanation would be helpful." Response: Added new Eq. 5, introducing the a priori covariance, Eq. 7a, introducing the bias, and Eq. 7b, the covariance of 7a. Updated wording, "Equation 7a is the predicted bias between x_c (the measured AIRS value) and x_aircraft_c (the aircraft value with the AIRS Averaging kernel applied), and is the expected difference of Eqs. 4 and 6b. Equation 7b is the covariance of Eq. 7a, and estimates the predicted error."

Equation 6, "Acb is not defined". Response: change Acb to GcKb.

Line 235, "Here the explanation should be given that this is because the retrieval vector

is log(VMR)." Response: updated. "Because the retrieved quantity log(VMR), the error in ppb is approximately the fractional error times the methane value in ppb."

Line 255, "Define validation error". Response: Now it is consistently called "validation uncertainty" throughout the paper rather than "validation error" and "validation uncertainty".

Line 259, "Where do these errors come from?". Response: These errors are now tied to equations.

Line 266, The reviewer notes that not only the stratosphere influences the troposphere, but the troposphere influences the stratosphere, due to the broad sensitivity. Response: Added sentence, "Similarly, the true state in the troposphere influences retrieved values in the stratosphere."

Line 282. Is the 16 ppb the larger of the two errors from model propagation? Response: We updated this to set the "validation uncertainty" to the average of the two model results, 10 ppb. This agrees with the previous result from Wunch et al. (2010).

Reviewer comment: How does the profile extension relate to the "validation uncertainty"? Doesn't it relate more to the bias estimate? Response: The profile extension obviously affects the bias versus validation data which affects the bias correction. However, it is most relevant to the uncertainty that results from extending the aircraft profile using a model. Text update, "Appendix A shows further analysis of mean differences of AIRS minus aircraft for different profile extension choices. The bias varies by $\sim$ 5 ppb for different profile extension choices when comparing at 700 hPa, $\sim$10 ppb for different profile extension choices when comparing at 500 hPa, and $\sim$11 ppb for different profile extension choices when comparing the column above 750 hPa."

Line 291. Reviewer requests that Worden et al., 2011 bias correction be summarized briefly. Response: Added text, "We therefore use the bias correction approach described in Worden et al. (2011), where a bias profile (which varies by pressure) is

passed through the averaging kernel to account for the AIRS sensitivity, as seen in Eq. 8. The form of the bias profile, delta_bias set by Eq. 9."

Eq 7. Reviewer wonders if A is a vector. Response: A is a matrix, as x-hat is a profile, as shown in Fig. 6. Text updated, "Where x = ln(VMR), because the retrieved quantity is ln(VMR), delta_bias is a vector, and A is the averaging kernel matrix for x = ln(VMR)"

Eq 7. Reviewer wonders about the handling of log. Response: text and equations updated to handle log consistently.

Line 315. Reviewer wonders why there is a bias peak about 200 hPa. Response: It seems that the bias is increasing through the stratosphere, whereas the sensitivity is decreasing above 100 hPa, and these two combine to generate a peak about 200 hPa. But this is speculation.

Section 4 title changed from "Evaluation against aircraft data by latitude" to "Evaluation against aircraft data versus latitude", because as the reviewer points out, there is no fitting of bias or skill as a function of latitude.

Line 319 Reviewer suggests wording update to, "Figure 6 shows a comparison between all AIRS measurements within 50 km and 9h of an aircraft measurement over the pressure range of the partial column measured by the aircraft.". Response: The wording was updated to, "Figure 5 [figure numbering update] shows a comparison between all AIRS measurements within 50 km and 9h of an aircraft measurement and the aircraft. The quantity compared is the partial column XCH4 VMR within the pressure levels measured by the aircraft."

Figure 7 legend unreadable. Response: Add text in the figure caption with the information in the legend.

Line 334-335, reviewer questions what the legend means, e.g. 0.0 +/- 4. Response: This was not well explained in the text previously. This is an estimate of the overall bias and uncertainty in the bias. Each campaign or station's bias is independently calculated

and then the mean and standard deviation are calculated. A new sub-section was added at the end of Section 4.1, "4.2.6 The bias and bias uncertainty The bias is estimated by calculating the mean bias for each campaign or station separately, then calculating the mean and standard deviation for all campaigns / stations. The bias versus HIPPO is 0 $\pm$ 4 ppb. The bias versus ATom is 3 $\pm$ 4 ppb. The bias versus NOAA measurements is 9 $\pm$ 7 ppb."

Reviewer wants "roughly the same location and time" defined in line 344. Response: Text added to clarify, "The bias component is approximately the same for all AIRS methane measurements taken on the same day within 50 km, as we do not expect large variations in temperature and water vapor errors over these scales, which we presume to be a driver of these correlated errors."

Reviewer says this sentence is hard to parse, "The number of AIRS observations averaged ranges from 9 to 53 and averages 20.". Response: This was updated to, "We average over 1 day, the AIRS observations matching a single HIPPO or ATom measurement, within +-50 km and 9 hours of the measurement. We specify that there needs to be at least 9 AIRS observations for each comparison so that the systematic error, and not the precision (or measurement error), is the dominant term. These daily AIRS averages contain, on average, 20 AIRS observations."

In Figure 9, the reviewer noted that the figure showed VMR but was indicated as a partial column. Response: This is an XCH4 partial column, as noted above and now explained in the paper.‘ The wording describing the partial column throughout the paper, to remove this confusion, is, "The partial column XCH4 VMR within the pressure levels measured by the aircraft".

365-375. The reviewer says that this section is hard to follow and needs explanation on the importance of the values shown. Response: Updated this text to indicate what the numbers mean, and what the findings are. Also separate into 4 new subsections, discussing daily, monthly, 3-month, and seasonal cycle averaging. Added a new section

on the bias characterization (in response to a previous comment.

The rewritten text is (the next 7 paragraphs):

"4.2.1 Daily average errors at TGC We look at daily averages versus aircraft data, and find a similar result as found with comparisons to Atom and HIPPO: daily averages have much larger errors than would be predicted if random errors are assumed. The standard deviation of (AIRS minus aircraft) at TGC is 24 ppb, the standard deviation for (daily AIRS average minus aircraft) is 11.5 ppb, as seen in Fig. 9a, and the predicted error for daily averages, assuming randomness in the error, is 6.0 ppb. Therefore, similarly to ATom and HIPPO, errors within 1 day and 50 km contain 11.5 ppb correlated error.

"4.2.2 Monthly average errors at TGC The aircraft measurements are usually taken about twice per month. The standard deviation of (monthly AIRS average minus aircraft) is 8.2 ppb (Figure 9b) for months containing more than 1 aircraft observation. This is compared to the daily error divided by the square root of the number of days averaged, 8.0 ppb. Therefore, errors for observations $\sim$2 weeks apart are uncorrelated.

"4.2.3 3-month average errors at TGC We average over 3-month scales, where averages must have at least 3 days. The standard deviation of (3-month AIRS average minus aircraft) is 6.2 ppb. The predicted error, taking the 11.5 ppb daily error and dividing by the square root of the number of days averaged, is 6.0 ppb. Therefore, errors for 3-month averages are $\sim$uncorrelated.

"4.2.3 Seasonal cycle average errors at TGC We average matched pairs within each month from any year. (AIRS minus aircraft) for these averages, have a standard deviation of 5.9 ppb, whereas the predicted error, from the daily average divided by the square root of number of observations, is 4.2 ppb.

"4.2.4 Summary of average errors at TGC To summarize, averaging AIRS observations within one day reduces the error versus aircraft, but correlated errors prevent daily av-

eraged errors from dropping below 11.5 ppb. Averaging daily averages over 1 or 3 months equals the daily error divided by the square root of the number of days averaged, indicating that errors are random in this domain. However, averaging months from multiple years, does not reduce the error below 6 ppb, either due to correlated errors, or validation uncertainty.

"4.2.5 Summary of errors at all NOAA aircraft sites Table A.3 in Appendix A shows the single-observation standard deviation for all NOAA aircraft sites. The ocean vs. land observations show similar values, with land and ocean standard deviations within 2 ppb. A single land observation has a standard deviation versus aircraft observations of 23 ppb for the partial column XCH4 VMR within the pressure levels measured from the aircraft, in agreement with predicted observation error of 23 ppb. The standard deviation for daily averages is 15.2 ppb. This can be compared to the predicted error for the daily averages, assuming randomness, of 5.9 ppb. This indicates that there are correlated (non-random) errors on the order of 15 ppb when averaging observations within 50 km and 1 day. The monthly standard deviation is 10.9, in reasonable agreement with the predicted of 9.4 ppb (from the daily average standard deviation divided by the number of observations averaged). The seasonal cycle average, which is a monthly average of all matched pairs from all years, has a standard deviation of 7.7 ppb, which is similar to the predicted error of 6.9 ppb (from the daily average divided by the square root of number of observations). We find that estimating the error as the daily standard deviation divided by the square root of the number of days averaged is a reasonable estimate of the actual error.

"4.2.6 The bias and bias uncertainty The bias is estimated by calculating the mean bias for each campaign or station separately, then calculating the mean and standard deviation for all campaigns / stations. The bias versus HIPPO is 0 ± 4 ppb. The bias versus ATom is 3 ± 4 ppb. The bias versus NOAA measurements is 9 ± 7 ppb."

Other changes:

Author institution updated for Edward J. Dlugokencky to "National Oceanic and Atmospheric Administration, Global Monitoring Laboratory, Boulder, CO, USA"

NOAA ESRL aircraft changed to "NOAA GML aircraft network" due to an updated name for this program.

Thank you to both reviewers for their helpful comments. We have responded to all reviewer comments.

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