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Atmospheric Measurement Techniques Discussions

Interactive comment on "Validation of the CrIS Fast Physical NH_3 Retrieval with ground-based FTIR" *by* Enrico Dammers et al.

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We would like to thank Referee #1 for his/her time, constructive and helpful comments and suggestions. Note, throughout the document R1 stands for reviewer 1, and figures named R1.x point to the x'th figure in "Reply to comments, Referee #1.

General comments:

1. Since the mean number of degrees of freedom of the NH3 retrieval for both instruments seems to be near 1, comparison of the total NH3-column amounts is a central part of the paper. However, some major retrieval characteristics should additionally be provided. Especially a kind of total column operator, like the one shown by Rodgers and Conner, 2003, Fig. 11. E.g. Fig 5 of the actual draft could be modified such that

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the AK for absolute concentrations or partial column amounts is provided.

We agree it would be a good idea to show total column averaging kernels, but with this version of the CrIS retrieval we did not save the required temperature and water vapour input profiles in the output retrieval files to compute accurate total column averaging kernels. In a future version of the retrieval output files we will compute and provide the total column averaging kernels to go along with the total column values. In the case of the FTIR retrievals, the partial column averaging kernel is provided in the datasets. Figure R1.1 shows the partial column averaging kernel for the example as shown in Figure 5.

2. Further, in Fig. 5 I wonder why the FTIR AK does not peak at the ground level: is there some problem with half-levels there? This should be explained in the paper. The FTIR averaging kernel does not seem to always have complete sensitivity for the ammonia near the surface and varies from observation to observation. As mentioned in the text it usually peaks in between the surface and 850hPa. The method seems to be slightly more sensitive for the second layer in the retrieval. Furthermore, one should take into account that we only have a total DOF of 1 for most observations. Hence one cannot expect a perfect AVK peaking at its own level. We point the referee to the Figures R2.1-R2.4 in our reply to Referee #2.

3. Also, while error estimations of the profile retrievals are presented, it would be helpful to have those numbers for the total column amounts as well. The estimated errors on the FTIR total column amounts are mentioned in section 2.2, being in the order of 30% for which we point you onward to Dammers et al., (2015). In case of CrIS we do not mention a specific percentage in the text, but most total columns have an estimated error in the order of 10 %. This estimate however is on the low side as it does not yet include an estimate for the systematic errors in the retrieval.

Specific comments:

4. L27-35: The abstract should be made more concise. These lines, which include

mainly motivation could be skipped. We removed Line 27-35, and edited the abstract to be more concise. Furthermore we made the following edits: Line 44: Added "(<1.0x1016 molecules cm-2)" Line 45: Removed "and the FTIR total columns are smaller than 1.0x1016 molecules cm-2," Line 46: Removed "are small with CrIS showing" Line 47: Added "show" Line 47: Removed "around +2.4 x 1015 (standard deviation = $\pm$5.5 x 1015) molecules cm-2, which corresponds to a relative difference of $\sim$+50% (std = $\pm$100 %)." Line 48: Added "The CrIS and FTIR profile comparisons differences are mostly within the range of the estimated retrieval uncertainties single level retrieved profile values showing average difference in the range of $\sim$20 to 40%" Line 50: Removed "for these comparisons" Line 51: Added "into the boundary layer that typically peaks at" Line 51: Removed "to" Line 52: Added "($\sim$1.5 km)" Line 52: Removed "and" Line 52: Removed "retrieved profiles also compare well with the" Line 53: Added "is" Line 53: Removed "of" Line 53: Added "std =" Line 53 Added "," Line 53 Removed "and a" Line 53: Added "%" Line 53: Added "std =" Line 54: Removed "Most of the absolute and relative profile comparison differences are in the range of the estimated retrieval uncertainties. However, t" Line 56: Added "At the surface, where CrIS typically has lower sensitivity," Line 55: Removed "he CrIS retrieval does" Line 55: Added "it" Line 56: Added "s" to "tends" Line 56: Removed "the concentrations in the levels near the surface at" Line 56: Added "under" Line 56: Added "conditions, and underestimate under higher atmospheric concentration conditions." Line 58: Removed ", most probably due to the detection limit of the instrument, and at higher concentrations shows more of an underestimation of"

We also made a number of small edits to improve the readability of the main text: Line 25: Edited the email address as the old one is no longer viable (change of institute) Line 71: Added "," Line 97: Added "can" Line 97: Removed "and" Line 107: Added "," Line 110: Added "," Line 192: Changed pseudo-lines to Cross-sections Line 442: Removed "which" Line 443: Added "," Line 445: Added "," Line 462: Removed "." Line 463: Removed "Because of" Line 463: Added "Due to" Line 608: Removed "and Jacob Siemons (ECCC)"

5. L39, L48-49: ‘compare well’ These are qualitative terms which do not contain much (if any) information content. Please try to avoid those throughout the manuscript and concentrate on quantitative assessments. Removed qualitative terms throughout the document. Line 30 (all line statements are the positions within the new document): changed “compare well with” to “have a positive”. Line 301: changed “The overall agreement is good” to “There is an overall agreement” Line 391: changed “good” to “high” Line 400: “removed well” Line 440: changed “agree quite well” to “show agreement” Line 473: removed “good” Line 523: changed ‘agree well with” to “ have” Line 526: changed “agree very well” to “are in agreement”

6. LL95-96: ‘However, the uncertainty of the satellite observations is still high due to a lack of validation.’ The reasoning is a bit strange: the uncertainty is not caused by lack of validation but rather the knowledge of the uncertainty.

Edited the sentence to “However, the overall quality of the satellite observations is still highly uncertain due to a lack of validation.”

7. LL245-246: ‘Do note that on average the observations have a DOFS between 0.9 and 1.1.’ Could you please provide a Figure or numbers of the DOF distribution of all measurements entering the comparison.

Figure R1.2 shows the distribution of the DOF of all measurements. Note that the <0.1 DOF are already removed from this set. $\sim$80 % of the observations have a DOF in between 0.9 and 1.1, with a median of almost 1.0.

8. L246: ‘clouds will implicitly be accounted for by the quality control’: What is the effect of a partially cloudy field-of-view? That’s a good point. Currently, there is a cloud filter in development to exclude clouded scenes in the future. In our case we remove all observations with a DOF of <0.1 which removes most of the clouded scenes (e.g. thick clouds $\rightarrow$ no ammonia observed). Besides a reduction in DOF we do not expect further major impacts as mentioned in the TES-NH3 retrieval paper (Shephard et al., 2011). As an example to illustrate potential effects (or the lack there of) we give Fig R1.3.

The figure shows a MODIS scene for northern Canada with both visible clouds and fire plumes. The bottom panel shows the calculated CrIS surface NH3 for the same period. As one can observe there are a number of hotspots for NH3 found for the observations surrounding the fires and of the plumes. The optically thick clouds are filtered out by our artificial cut off. The remaining retrieved concentrations for observations with partially covered and by optically thin clouds do not show any strange patterns or alternating high and low retrieved concentrations.

9. L301: 'total column comparison': Has this comparison been performed with or without the application of the FTIR-AK as described in chapter 2.5? Since the FTIR is generally better suited for total column retrievals due to its better sensitivity nearer at the ground (where most of the NH3 is present), I doubt that the transformation like in Eq(1), L278 is helpful. Here the better instrument (FTIR) should be transformed to the worse (CrIS) to compare with the CrIS total column amounts. I.e. there should be Figures like Figs. 2 and 3 with the raw data and after the transformation as just described.

The total column comparison has been performed with the application of the FTIR-AK as described in chapter 2.5. In principle we agree that the better instrument should be transformed to the worse (CrIS). However, we wanted to keep the study comparable to the IASI validation study, and thus apply the AVK in the same manner as done in that study. The IASI product does not produce an averaging kernel and thus we cannot apply the satellite observational operator in both cases. Furthermore, to meet readers who would rather see it the other way around, we added alternative figures transforming the FTIR profiles with the CrIS AVK, which are shown in figures A5, A6 and A7.

10. L318: 'In Toronto, Bremen and Pasadena there is good agreement' In case of Pasadena, I would not call the agreement good. Please also avoid this qualitative terms. Changed the qualitative terms as mentioned in edit number 5.. We also added some lines on the results at Pasadena and Wollongong, see edit number 13 for the full

description. Removed, “Pasadena”,

11. L319: ’and low bias in the CrIS total columns for intermediate values’ This seems not to be the case for Bremen. The only outlier for Bremen is the value that is marked as an outlier by the three sigma filter as used in Figure 2. Furthermore the number of observations is too small for any good statistics. Added “except for the outlying observation in Bremen, which is marked as an outlier by our three sigma filter used for Figure 2.”

12. L322, Fig. 3: Could you also discuss in the text what the reason for the apparently systematic deviations at Wollongong may be. There are a number of reasons why the Wollongong bias might look higher than the others. The first is the date of observation. The two comparisons with the highest CrIS to FTIR ratio were both made during the end of November in 2012 when there were multiple fires occurring in the surrounding region (GFED4.1s). Possibly the CrIS footprint covers the plumes from the fire, which was not observed by the FTIR due to an (for us) unfavourable wind direction. The remaining comparisons on average show a MD of $\sim$ 5 x 1015, which is similar to our station wide result. Another explanation might be the difference in observed air masses which can be larger for coastal sites (e.g. Wollongong, and essentially Toronto). Depending on the wind direction there is either clean air coming in from above the lake/ocean which will mean there is a reduction in FTIR observed NH3 while the satellite potentially observes above land. Vice versa observations from the satellite above the ocean/lake can be far lower than the columns observed by the FTIR with a wind direction coming from an inland direction. This heterogeneity is also visible for sites with larger gradients in orography, such as Pasadena and Mexico City.

Line 311: Added “Similarly to Mexico City the comparison also shows an increase in scatter for Pasadena, where the FTIR site is also located on a hill.”

Line 315: Added “In Wollongong, there is less agreement between the instruments. There are two comparisons with large CrIS to FTIR ratios while most of the other

comparisons also show a bias for CrIS. For both cases the bias can be explained by the heterogeneity of the ammonia concentrations in the surrounding regions. The two outlying observations were made during the end of November, 2012, which coincides with wild fires in the surrounding region. Furthermore the Wollongong site is located coastally, which will increase the occurrences where one instrument observes clean air from the ocean while the other observes inland air masses."

13. L331, Fig. 4: 'show the standard deviation for each value' Is this the standard deviation of the distribution of the differences or the standard error of the mean difference (i.e. the former divided by sqrt(number of values))? The latter should (also) be shown to detect any significant measurement bias. Fig 4 showed the standard deviation of the distribution of the differences. As noted in the reply to Referee number 2 we edited the figure to show the 95% confidence interval i.e. $\sim$2x standard error.

14. LL379-380: 'along with the shorter atmospheric path lengths for observations from the ground-based solar-pointing FTIR' Could you explain, why the FTIR path length is shorter compared to the satellite? Is this always the case? In principle the atmospheric path length should be more or less similar. The path length of both instruments vary per location of the site, time of day and field of view of the satellite, but the difference should be more or less near zero.

Line 379: Removed sentence

15. LL377-385: As already mentioned, for this discussion the total column operator or the partial column(number density) AK would be interesting. As the FTIR is more sensitive down to the ground level than the satellite where there are highest concentrations of NH3, the satellite retrieval should be determined by the a-priori there. So the higher column amounts may be produced by higher a-priori values at the ground. That's a good point but for the fact that the application of the observational operator should reduce the effects of the difference in sensitivity and a-priori choice. Any remaining effect of the a-priori is hard to judge without a repeat of the retrieval. What potentially can be

done to further reduce the influence of the a-priori is switching out the a-priori. For a number of examples of the a-priori switch, we point you to figures R2.1 to R2.4 in our reply to Referee number 2.

16. L550: 'improvements to the NH3 line spectroscopy to reduce the uncertainty coming from this error source' Could you give the information if the CrIS retrieval also uses Hitran2012, like the FTIR? The CrIS retrieval also uses HITRAN 2012.

Added: "and uses the HITRAN database (Rothman et al., 2014) for its spectral lines"

Technical comments: L566, Fig. A1: the arrangement of the panels in the figure is transposed with respect to the description in the caption. Good catch, L566 Fig. A1 caption, changed to: "Error profiles for each of the error terms. The left panels show the random errors, the right panels the systematic errors. The top two panels show the error in VMR. The bottom panels show the errors in partial column layers [molecules cm-2]. (See Figure A.2 for the same figure but with the errors relative to the final VMR and partial columns per layer)"

L571, Fig. A2: same problem as in Fig. A1. Moreover, the top and the bottom row seem to show identical data. It is correct that the top and bottom row are showing identical data as the error is initially derived for the VMR value and subsequently applied to the partial columns.

L571 Fig. A2 caption, changed to: "Relative error profiles for each of the error terms. The left panels show the Random errors, right panels the Systematic errors. All four panels show the error in a fraction of the original unit used in Figure A1. (See Figure A.1 for the same figure but with the absolute errors)"

References. Shephard, M. W., Cady-Pereira, K. E., Luo, M., Henze, D. K., Pinder, R. W., Walker, J. T., Rinsland, C. P., Bash, J. O., Zhu, L., Payne, V. H., and Clarisse, L.: TES ammonia retrieval strategy and global observations of the spatial and seasonal variability of ammonia, Atmos. Chem. Phys., 11, 10743-10763, doi:10.5194/acp-11-

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van der Werf, G. R., Randerson, J. T., Giglio, L., van Leeuwen, T. T., Chen, Y., Rogers, B. M., Mu, M., van Marle, M. J. E., Morton, D. C., Collatz, G. J., Yokelson, R. J., and Kasibhatla, P. S.: Global fire emissions estimates during 1997–2015, Earth System Science Data Discussions, doi:10.5194/essd-2016-62, in review, 2017.

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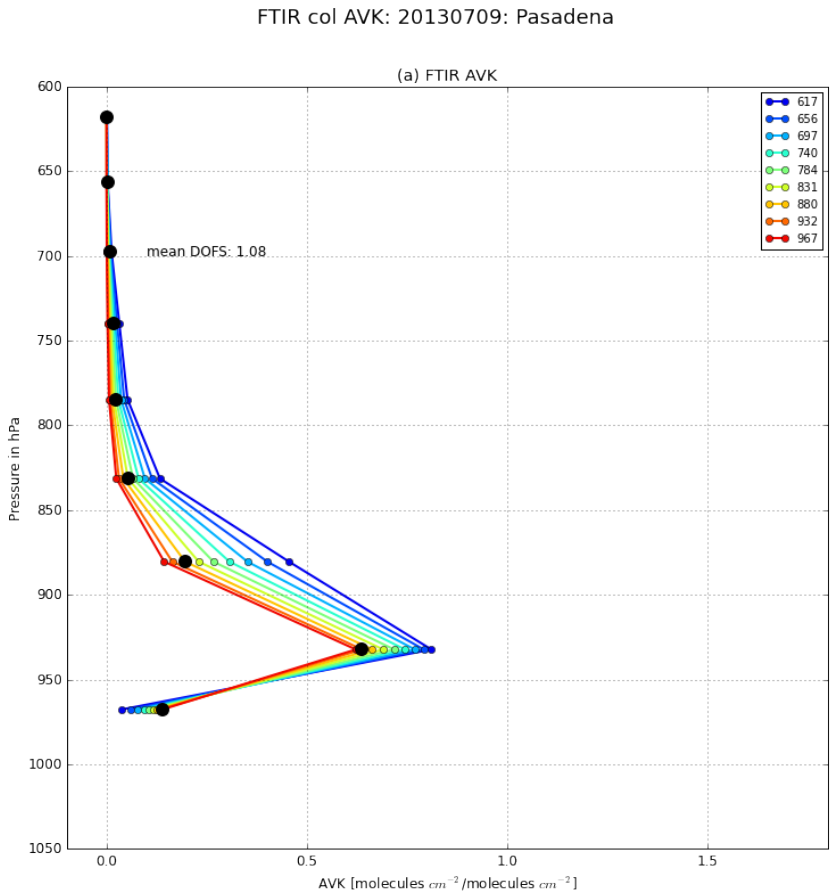

Fig. 1. FTIR averaging kernel in [molecules cm-2 / molecules cm-2]. The black dots show the matrices diagonal values.

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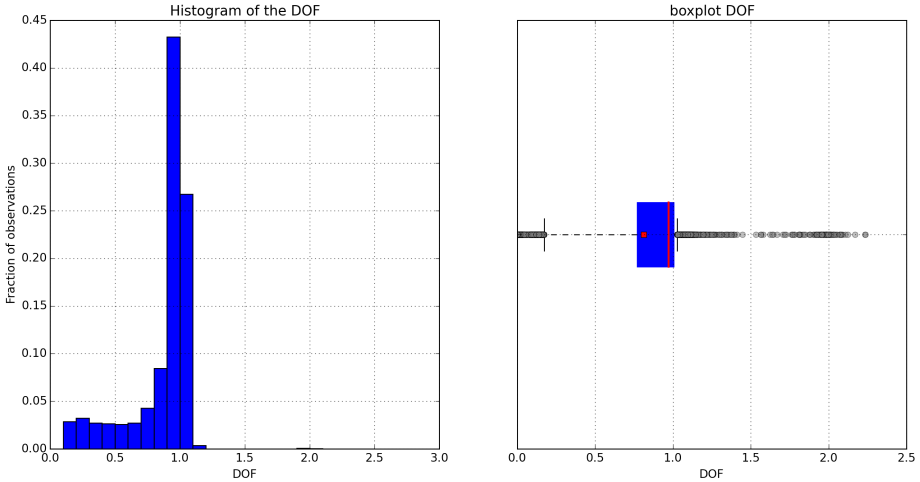

Fig. 2. Distribution plots of the DOF of all CrIS observations used in this study. The left panel shows the fraction of all observations for each specific DOF range. The right panel shows a boxplot of the sam

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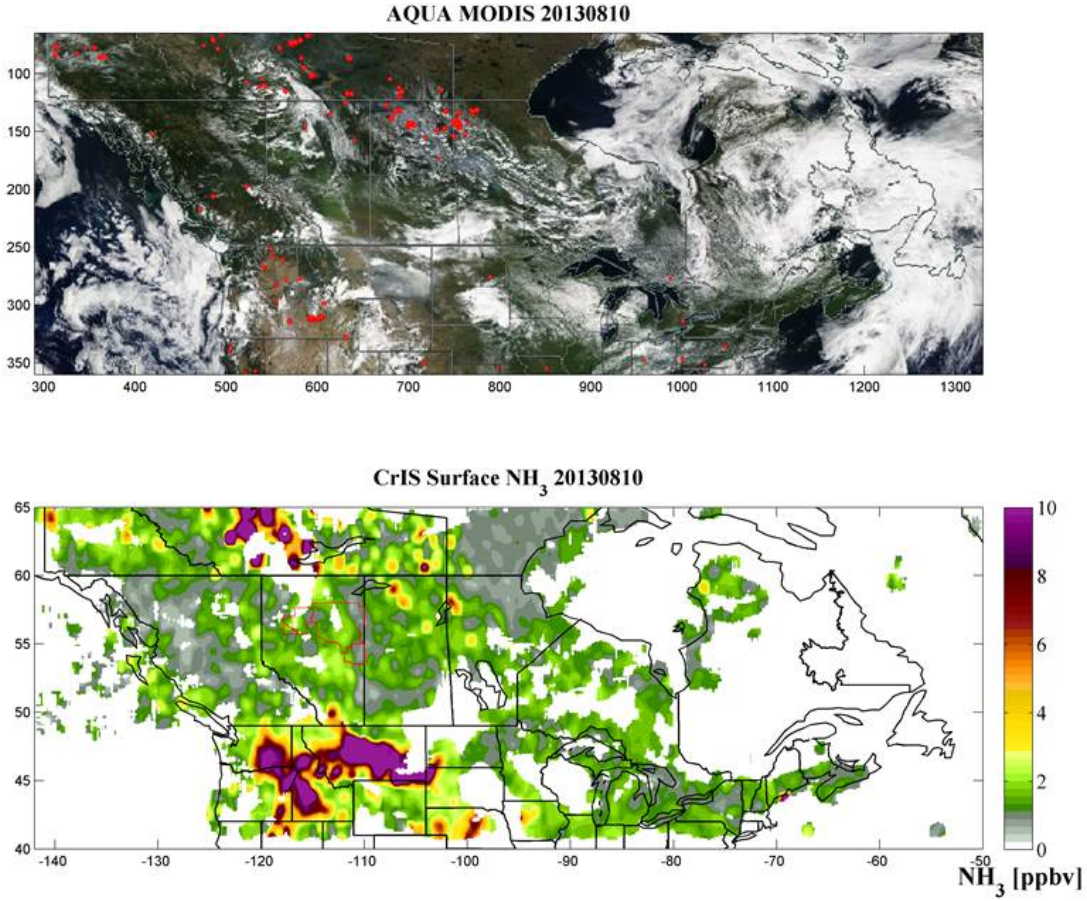

Fig. 3. Top panel shows the MODIS image over Canada on the 10th of August 2013. Bottom panel shows the retrieved CrIS surface concentrations for the same day.