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Interactive comment on "Validation of ACE-FTS version 3.5 NO$_y$ species profiles using correlative satellite measurements" *by Patrick E. Sheese et al.*

Anonymous Referee #3

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General Comments

This paper describes the validation of NOy species measured by ACE-FTS versus previous versions as well as several satellite datasets. The introduction needs work: the authors sometime show the reactions involved and some time they do not. They have to be more consistent. I strongly encourage them to show all the reactions. The methodology and datasets are presented in a verbose manner that could be more succinct. The figure shown for each species are inconsistent. For some the authors shown profiles, then differences, then seasonal biases, then hemispheric biases and for others a subset of these.

I recommend another review after addressing the comments below.

Major comments:

Printer-friendly version

Discussion paper

A figure showing the diurnal variability for the NOy species used in the study needs to be shown. This would help the reader know when to expect a big impact due to this correction. See for example, Khosravi et al. 2013 Figure 2. (the figure can be normalized to be able to show all the species in the same figure)

The authors needs to include the errors (a combination of the precision and accuracy) for the datasets. This would allow the reader to see if the differences between the datasets are significant or not.

The author needs to add a figure showing the fake kernels constructed with the normalized Gaussian distributions against the kernels of the satellites that do provide kernels (at least MLS and MIPAS). Also the author needs to add a figure showing that the results of applying both kernels (the faked and the actual kernels) are similar. The impact of averaging kernels is crucial in this type of comparisons.

Also, why not used the actual kernels when available and the fake kernels when not?

Comments:

P1L31: NOy also includes [N] (See Brausser and Salomon)

P1L36: The authors do not show the instrument average mean relative difference in figure 4, where do these estimates came from?

P2L1: for NO2, add "and up to 40% elsewhere." For HNO3 add "and up to 20% at 30-40km" Add a summary for the N2O5 evening.

P2L2: For ClONO2 add "and varies from -20 to 15% from 13 to 20km"

P2L6: NOy also includes [N] (See Brausser and Salomon)

P2L11: Not really a major role, that's ClO and BrO.

P2L14: This is not a detailed description of NOy chemistry. It is missing reactions for HNO4, NO3 and BRONO2. The authors should change this line to "A description of

the chemistry of the molecules validated in this study is shown below [Brausser and Solomon, 2005]" or something similar. Or, show the complete NOy chemistry.

P2L20: Add N2O + hv (lambda <= 200nm) - > N2 + O1(D) R. 5.129 Brausser and Solomon, (2005) (from now on BS05 reaction numbers refer to the Third revised and enlarged edition)

P3 R4 is missing the (3P) that is O(ˆ3 P)

P3L3 delete this line, not relevant to this paper.

P3L5 HNO3 sources add reactions 5.151 (and keep 5.152 R5 in the paper) HNO3 sinks add reactions 5.153 and 5.101

P3L9-11: Delete this paragraph not relevant to this study

P3L14: Add reactions 5.149a, 5.149b and 5.150 BS05

P3L17: Add reactions 5.159a and 5.159b BS05

P4 L15: Why HITRAN 2004? Why not HITRAN 2012?

P4 L17-20: Could you explain briefly how the new microwindows were selected? Did you use propagation of random noise and select microwindows that maximize information content or degrees of freedom? Did you minimize total error (precision and accuracy)? Etc...

P4 L20: Why the exclusion of ClO?

P5L6: What happen between 64 and 94km?

P5 L17: Why only one spectral window? Wolf et al. 2008 used two.

P5 L24: The authors state "ACE-FTS N2O5 typically exhibited a low bias on the order of 30% ..." This sentence only applies for daytime, during nighttime the biases were worse, in the order of 50% for uncorrected and around 35% for corrected.

P6 L1-4: Wolf et al 2008 states: That MIPAS and ACE-FTS agree within 1% (not 5% as the author states) between 16 and 27km and that ACE-FTS has a positive relative bias of 14% (not 20% as the author states) between 27 and 34 km.

Section 2.1.1: The authors need to specify if the interfering species were retrieved or if their concentrations were set to climatological values. Did the retrieval used the O3 and H2O previously retrieved to constrain their impact, etc?

P7 L1: the diurnal variations along the line-sight in the NO2 retrieval algorithm also affected ACE-FTS NO2 retrievals but the author forgot to mention it.

P7L17: Add O2.

P7L18: the spectral range is 248-956nm See table 1 of Kyrola (2004).

P8 L12: five spectral bands (not channels)

P8 L16: an anomaly occurred in the interferometer mirror slide mechanism (not the instrument drive unit).

P8 L25: Change Hanke, 1997 for Levenberg (1944) and Marquardt (1963)

P9 L2: the authors need a citation for the a-posteriori regularization.

P9 L6: without pushing the results towards an a-priori profile (Neither the ESA one but the authors did not mention it)

P9 L10: As well, the forward model . . . → Further, the forward model can allow deviations from LTE which have an impact in the mesospheric retrievals.

P13 L13 Waters citation should follow MLS not Aura.

P13 L18: the authors did not mention the ascending node time for the other satellites (MIPAS, GOMOS, SCIAMACHY, etc)

P13 L20 temperature, GPH, concentrations of over 15 ... and cloud ice.

P13 L23: radiometer not channel P15 L25: radiometer not channel

Section 2.4: this is not the latest version for the MLS data. If the authors are not going to use it at least it should state that it exists. MLS version 3 was adversely impacted by clouds leading to noisy HNO3 in the UTLS. The adverse cloud impacts were substantially mitigated in version 4 (Livesey 2015).

P16L5: MLS also uses the JPL spectral catalog.

P16L10: Why only from band C? The authors should include both or an average or indicate why HNO3 band A was not used.

Also, the authors did not mention that SMILES covers the entire diurnal cycle in a period of about 2 months. A great plus of this dataset!

P17L19: Use sigma symbol (in latex \sigma for example)

P18L5: Please add the equation for the standard deviation of the relative differences instead of explaining with words.

P19L9-10 Why Sander et al (2003). That kinetics file have been superseded. The one the authors used is the evaluation number 14 while the newest one is 18. The author at least needs to check that no new rate constants have been recommend for the most important NOy and O3 reactions.

P20L13: The difference are much worse because both versions retrieved closed to zero values.

P21L17: What is meant by statistically significant? 95% confidence more than 3, 10, 100 please explain.

P21L23-24 Why do the number of coincidences drop at some altitudes? Please explain.

P22L23: Why did the comparison with MIPAS did not improve when using the diurnal

C5

scaling? ACE-FTS measures at sunset/sunrise while MIPAS measures at around 10, this should make a difference, unless the diurnal variation is flat.

P23L10-23: Please explain the top row of the figure without mention any seasonal bias. Then, mention that due to ACE coverage and MIPAS NO sensitivity there is only data during . . . Then explain the bottom row. Also, is there any reason to expect the comparison to work better over the summer months. Is the winter data wrong? If so, which data MIPAS or ACE.

P26L15 Where is the figure showing the profiles? As Figure 3,6 and 10.

Section 4.2.4: The authors should try to explain the much worse agreement found during the evening. Also, they need to explain a bit better the intention and the results of Figure 15.

Section 4.2.5: There is no profile figure for morning and evening. Please be consistent with the figures shown among the species.

P18L25: in line 15 (same page) the authors mention that the results for all species except for HNO_3 were improved by diurnal scaling. Now the authors state that for NO the diurnal factors did not help improve the comparison results. Please clarify.

Table 4 should also include NO no summer months and N_2O_5 evening

P29L2: In the comparison shown for NO, v3.5 still seem to have bias as big as 10% in this region. The -6% bias was versus MIPAS. So, it seems there was no improvement.

P29L4: The authors said that the bias was -6% and now they state approximately -5% (just a few lines apart). Please choose one. Also, add a statement: Above 40km, the bias is up to 40%.

P29L10: Following figure 8 the statement that start "with diurnal scaling . . ." seems to be wrong. Something like: "With diurnal scaling, this negative bias varies from $\sim$-10% to 3% for evening comparisons... and from -12% to 40% for morning comparisons

between 20 and 40 km." will be better.

P29L13: please clarify where do this statement ("In the 14-25km . . .) came from. Figure 8 stops at 20km and figure 7 includes all the satellite datasets. Also,

P29L12: Did the characterization of the lineshape changed from V2 to V3? If yes, how?

P29L19: How can this be an improvement if v2 was within 20% and v3 can change up to 40%.

P30L4: Did you check the apriori profiles? Is this just speculation? If it is, the author's need to change the language to reflect that.

Figures: Titles should use subscripts. Also, the authors should use either 10ˆ-6, 10ˆ-9 or 10ˆ-12, that is to say, ppmv, ppbv or pptv, respectively.

In the caption first caption, the author should specify the values of the dashed lines added for clarity.

Delete Figure 2 and add a caption on each of the following figures.

Figure 1: Presumably the authors shown v3.5 – v2.2 rather than v2.2 – v3.5

Figure 2: change MIPAS___IMK to MIPAS IMK/IAA Also SCIA to SCIAMACHY where needed.

Figure 4: The two panels should be merged and a instrument average mean line (black thick line) should be added. Caption should state ACE-FTS – INST rather than ACE-FTS – HALOE.

Figure 5: Caption should state: mean relative difference profiles (ACE-FTS - MIPAS IMK/IAA)

Figure 8: Caption could say: Note that the occultation instruments have been excluded.

Figure 10: MIPAS__ESA and MIPAS___IMK need to be changed to MIPAS ESA and

MIPAS IMK/IAA

References:

Khosravi et al. 2013, doi: 10.5194/acp-13-7587-2013

Levenberg (1944), A method for the solution of certain non linear problems in least squares, Quarterly of applied mathematics, 2 , 164-168

Marquardt (1963), An algorithm for least squares estimation of nonlinear parameters, Journal of applied mathematics, 11, (2), 431-441

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Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2016-69, 2016.