

# Comparison between the assimilation of IASI Level 2 retrievals and Level 1 radiances for ozone reanalyses. Reply to referee # 2

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## 1 Reply to general comments

We thank the anonymous reviewer for his comments that helped to improve significantly the original manuscript. Detailed replies to his comments follow:

1. *The authors document clear differences between L2 and L1 assimilation, and seem to suggest that L1 assimilation should be considered. However, it seems to me that L2 with an improved a-priori may be a possible alternative to reach a similar performance of the analysis. Would running the IASI L2 retrievals with a varying a-priori, for instance taken from the Copernicus Atmosphere Monitoring Service daily analyses, be a feasible option? Would that solve part of the problem with L2 compared to L1? Could the authors discuss this in a more balanced way in the conclusion section (and maybe in the abstract as well)?*

### Answer:

The reviewer is right about the fact that L2 O<sub>3</sub> retrievals can be improved through a better a-priori (see reply n 3 for more details), and using O<sub>3</sub> forecast fields from Copernicus Services might represent a particularly valuable option for L2 production itself. We think that such option could reduce the differences between L1a and L2a in our experiments. However, more generally, the same question raised by our study concerns also models within the Copernicus services themselves (e.g. C-IFS). To assimilate L2 O<sub>3</sub> profiles in C-IFS we would then need to: i) run a first analysis/forecast excluding all IASI O<sub>3</sub> channels ii) run the L2 processor iii) run a second analysis/forecast cycle including only IASI L2 retrievals. On top of the extra numerical cost of such a system and practical difficulties when many instruments are assimilated, this could introduce error correlations between assimilated observations and model forecast that are not yet considered in DA algorithms. Another issue arises for spectral channels that are sensitive to multiple model variables (e.g. T and O<sub>3</sub>): splitting the DA problem in different steps (e.g. 4D-Var for T plus 1D-Var for O<sub>3</sub>) would result in the same observation to be used twice and might lead to different solution than solving the full problem at once (4D-Var). We have not investigated these aspects in our study and we cannot give final words on the best choice between L1 and L2 assimilation based only on our results in such a context. However, the ensemble of our results plus all the previous

arguments suggest that the L1 assimilation should deserve higher consideration, especially in the context of coupled systems such as the Copernicus Monitoring Services. Therefore, in general we prefer not to suggest an upgrade of the L2 processor with modeled a-priori for the scope of further assimilation. We included these elements in the revised conclusions (page 19, line 11).

- 5 2. *Although the L1 and L2 experiments are set up with as much as possible equal inputs and RTM (but different a-priori), there are still subtle differences as discussed in the text. I am wondering how much those differences may also result in differences in performance as documented in the paper? Especially since the differences documented between L1 and L2 are quite small. This leaves me with a bit an uneasy feeling that the results are maybe not fully understood.*

**Answer:**

10 Following the comments of the 1st referee we repeated all the experiments using exactly the same version of the radiative transfer for L1a and L2 retrievals (RTTOV 11, see reply n 1 to the 1st referee). We also verified if the differences on the meteorological profiles and surface skin temperature between L1a and L2 retrievals did not impact our results (reply n 2 to the 1st referee). This reduced further the possible sources of differences between the two approaches, which are now limited to: the a-priori, the vertical resolution and the minimization (3D-Var for L1a versus 1D-Var+3D-Var for L2a).

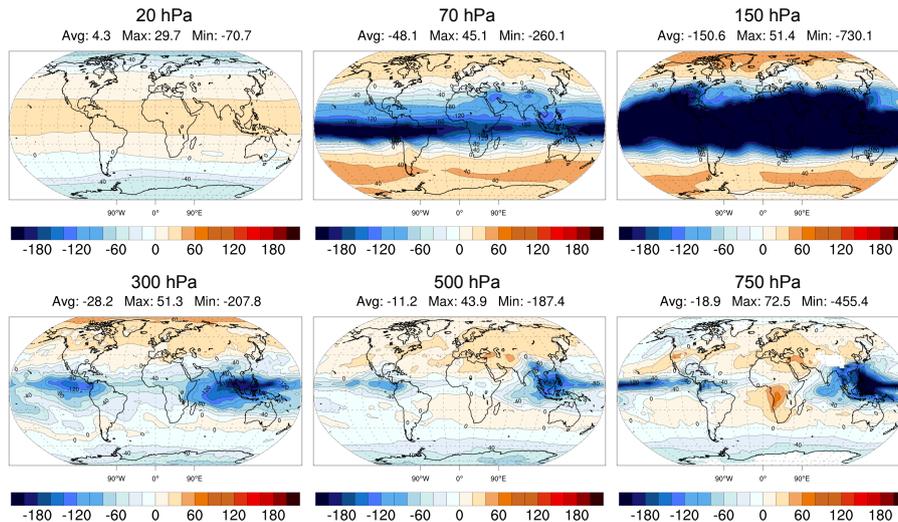
15 Although the L1a-L2a differences are now much reduced in the SH mid-latitudes (original differences were due to the radiative transfer), the new results still show significant differences between L1a and L2a at low latitudes (as high as 30%). We report in Fig. 1 the average difference between the control simulation and the SOFRID a-priori, which show that departures are very large (> 50% and as high as 700%) only at low latitudes. Differences in percent are very large close to the tropical tropopause (150 hPa) because the SOFRID a-priori is representative of mid-latitudes. However, we

20 remark that differences larger than 100% exist also in the free troposphere (300 to 750 hPa). Hence, Fig. 1 confirms that differences within data assimilation arise only when the L2 a-priori is strongly biased (i.e. at low latitudes, see also reply n 32) and strengthens the interpretation of the results given in the original manuscript. We included Fig. 1 in the discussion section (Sec. 4.1) and updated the conclusions of the revised manuscript (page 19, lines 5-8). We think that with these new elements the interpretation of the results is now more robust.

- 25 3. *The relative differences in Fig. 2 seem to indicate persistent biases. Maybe it is a lot of extra work, but I wonder how the difference plot of L2 retrievals for the climatological a-priori (presented in the paper), compared to L2 retrievals with MOCAGE profiles would look? Such a plot would be a valuable addition. Would that show similar features as in Fig.2, at around 300-500 hPa ?*

**Answer:**

30 An evaluation of SOFRID retrievals using an a-priori issued from a model was performed prior to this study and was actually the main motivation for this work. Indeed, results showed significant differences in the L2 tropospheric columns with the modeled a-priori and a better agreement with independent data (Fig. 2). Differences between the two SOFRID datasets seem qualitatively coherent with the L1a-L2a plot in the revised manuscript (increased O<sub>3</sub> at 300-500-750



**Figure 1.** Relative differences (%) between control simulation and SOFRID a-priori (divided by the correspondent O<sub>3</sub> values of the control simulation) averaged on July 2010. From left to right different pressure levels are displayed covering the stratosphere (top) and the free troposphere (bottom). Average, maximum and minimum values of the displayed fields are given on top of each map.

hPa). However, these experiments were based on a different model configuration (linearized chemistry) with degraded resolution (10°x20°). This preliminary analysis was also limited to tropical latitudes and integrated O<sub>3</sub> columns were evaluated without considering averaging kernels. Differently from our manuscript, the above analysis is focused on the L2 retrievals themselves (without further assimilation) and is still under finalization (comparison with radiosoundings). It will be presented in a separate paper once it is finalized and we prefer not to include partial results in our manuscript. In particular, the analysis of averaging kernels cannot be neglected when the assimilation is concerned, which limits the interest of Fig. 2 for our manuscript. Even so, we added a sentence in the conclusion (page 19, lines 12-13) to link these preliminary results to our study.

5

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4. *It would be helpful if the authors could add an image of the IASI averaging kernels, typical examples or averages, for NH, tropics and SH. In this way the reader can better understand at which pressures one may expect an impact of IASI.*

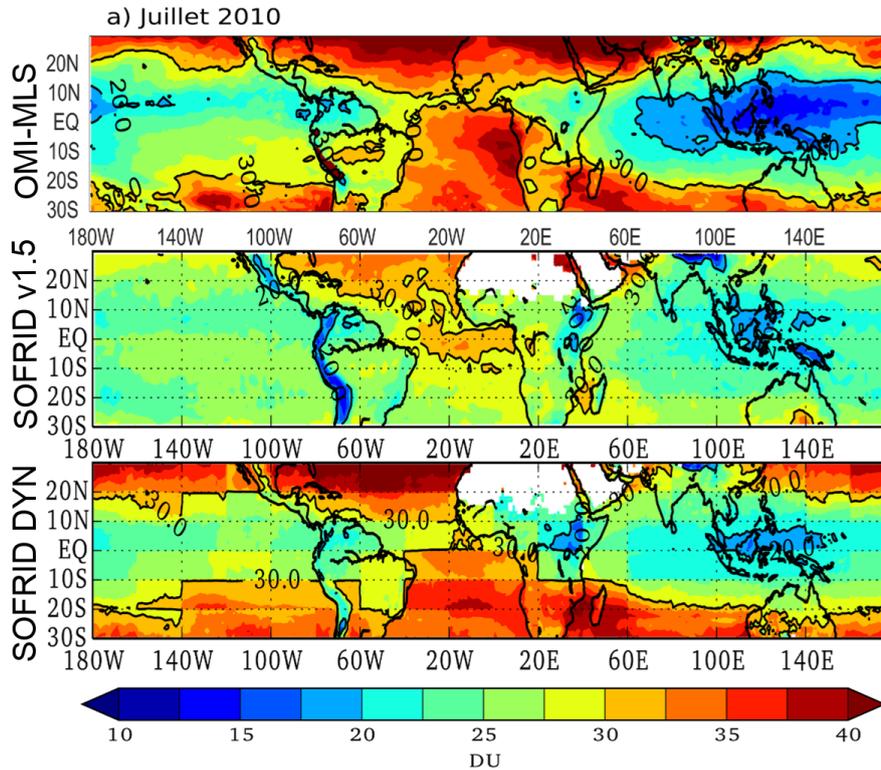
**Answer:**

We report in Fig. 3 the average kernels of the SOFRID retrievals for the month of July 2010, averaged globally and by latitude band. We included this figure in the revised manuscript and added the relative discussion (Sec. 2.1.2).

15

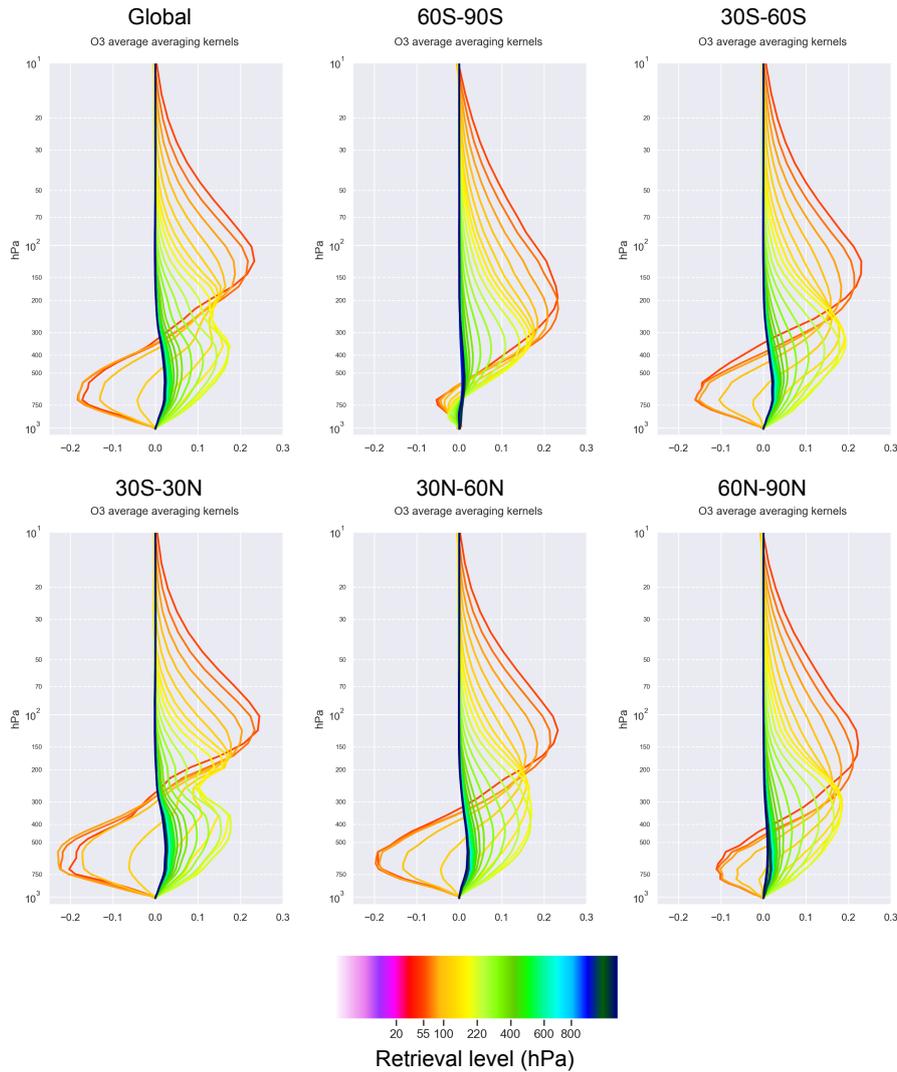
5. *The impact of IASI in both the L1 and L2 experiments seems to be relatively small, with also negative impacts. Especially when MLS is included as well, which already removes most of the bias around 200 hPa. This baseline ...*

**Answer:**



**Figure 2.** Average O<sub>3</sub> tropospheric columns (1000-100 hPa) from OMI-MLS residual method of Ziemke et al. (2011) (top), SOFRID v1.5 standard retrievals (middle) and SOFRID retrievals issued from a modeled a-priori (bottom).

5 The question of the reviewer being incomplete, we suppose that he/she raises some doubts about the practical benefits of assimilating IASI on top of MLS for O<sub>3</sub>. MLS assimilation is able to well correct the upper troposphere O<sub>3</sub> but, as Fig. 4 and 5 show, there is a significant positive correction of IASI in the tropics that MLS cannot perform. Also, MLS is on-board Aura satellite, which is already well beyond its mission's lifetime, whereas IASI and its successors will be flying for the next decades. We demonstrated in this and previous studies (Emili et al., 2014; Peiro et al., 2018) that the family of IASI sensors is valuable for data assimilation of tropospheric and lower stratosphere O<sub>3</sub>. This study provides further elements that we believe are important before implementing IASI O<sub>3</sub> assimilation in operational systems. We updated the conclusions at page 19 lines 20-22 to remind the importance of assimilating MLS in the stratosphere.

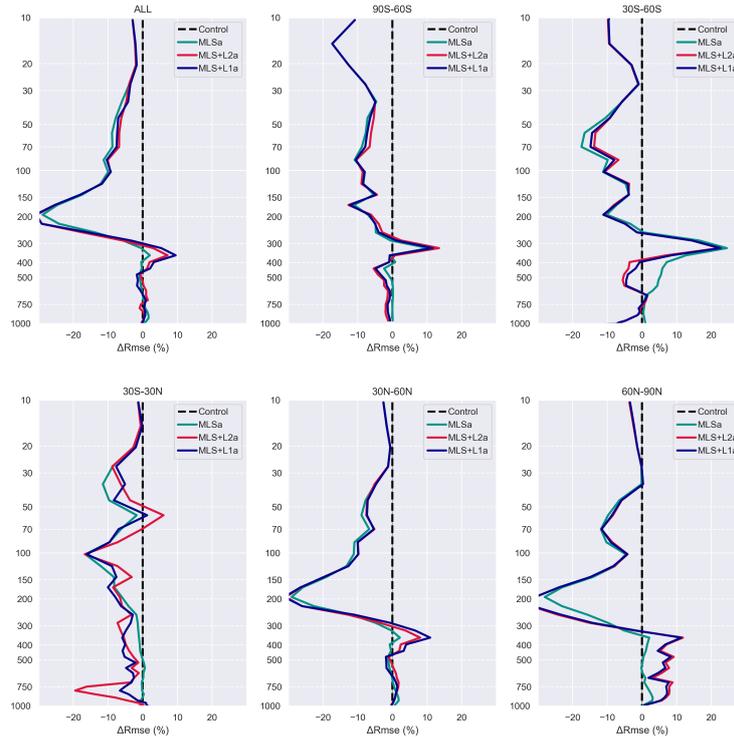


**Figure 3.** SOFRID O<sub>3</sub> averaging kernels for the month of July 2010 averaged globally (first plot) and for five latitude bands separately (90°S-60°S, 60°S-30°S, 30°S-30°N, 30°N-60°N, 60°N-90°N). Each coloured line corresponds to a retrieval's level, the corresponding pressure is indicated in the colorbar. Only SOFRID levels with a pressure > 50 hPa are displayed for better clarity.

## 2 Reply to specific comments

1. Title: "for ozone reanalyses": upon first glance this seems to suggest that the paper presents results of a multi-year reanalysis, which is not the case. Is it necessary to include the word "reanalysis" in the title?

**Answer:**



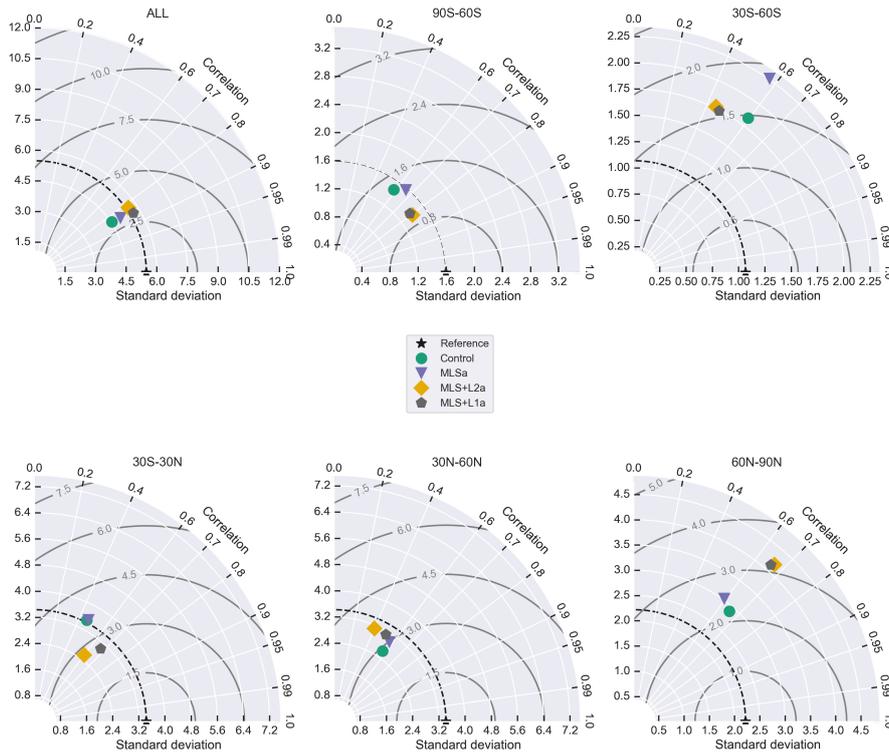
**Figure 4.** Relative difference of RMSE with respect to radiosoundings for MLS-a (teal), MLS+L1a (dark blue) and MLS+L2a (red). This figure replaced Fig. 6 of the original manuscript.

We used the word “reanalyses” because we presented only DA analyses in this study (instead of forecasts). However, we recognize that the study is mostly methodological and does not present results from long simulations. Therefore, we changed the title to “Comparison between the assimilation of IASI Level 2 ozone retrievals and Level 1 radiances in a chemical transport model” to avoid wrong expectations.

- 5 2. *Abstract, l9: "significant differences". The abstract does not give a very firm conclusion. Does the work presented justify the stronger statement that the non-linearity in the retrievals in combination with unrealistic a-priori profiles are the cause of the L1-L2 differences?*

**Answer:**

10 Although the results suggest that this seem the case we prefer not to give such a stronger statement in the abstract (and conclusions). The reason is that we did not evaluate explicitly the linearization error of the RTM in our study. Since



**Figure 5.** Taylor diagrams of modeled tropospheric ozone columns (340-750 hPa) for the Control simulation (green), MLS-a (violet), MLS+L1a (grey) and MLS+L2a (yellow) averaged globally and for five latitude bands separately. The Taylor statistics are computed against radiosoundings. This figure replaced Fig. 7 of the original manuscript.

RTTOV is already based on the linearization of a full line-by-line RTM (Saunders et al., 2018), doing this evaluation properly would require implementing the original RTM used by RTTOV in the CTM, which was out of the scope of this study. The main objective of our study was instead to provide some practical answers that can guide future developments for IASI assimilation.

- 5 3. *Abstract: Is there a clear recommendation from this work? Would L1 assimilation be preferred? A more clear statement would be helpful.*

**Answer:**

Our results indicate a slightly better variability of the tropospheric O<sub>3</sub> column when assimilating L1 data (Fig. 5). We included this element in the abstract. We also gave different arguments that promote L1 assimilation in the introduction

and in the conclusions (see also Reply n 1), but those are not a direct outcome of our simulations and we prefer addressing the reader to the conclusions to avoid a too lengthy abstract.

4. *Page 2, 15: Useful to mention the averaging kernels as well: .. and DOF linked to the averaging kernels ...*

**Answer:**

5 The sentence has been changed according to the suggestion of the reviewer.

5. *Page 2, 19: "First atmospheric composition models": Reformulate*

**Answer:**

The sentence has been reformulated.

6. *Page 2, 119: "However, some aspects of the Data Assimilation (DA) approach differ between the chemistry and meteorology communities." Please be more specific, or remove the sentence.*

10

**Answer:**

The sentence was removed.

7. *Page 2, 123: "This resulted necessary to avoid"; please reformulate.*

**Answer:**

15 The sentence has been reformulated.

8. *Page 2, 124: About the historical background: I was wondering about the problems encountered when assimilating L2 retrievals in NWP (paper of Eyre)? Is it the non-linearity and a-priori dependence (as suggested by the text), or is it a simplification of the retrieval results? The latter could arise when e.g. kernels and full covariance matrices are not used in the assimilation, or not provided by the retrieval teams, which would clearly lead to strong a-priori dependence of the analyses.*

20

**Answer:**

No mention to the averaging kernels was found in Eyre et al. (1993), which suggests that their difficulties arise from the simplification of the retrievals (missing use of averaging kernels). The sentence has been updated to make this point clearer (page 2, line 29).

9. *Page 2, 127: I would suggest to refer to the book of Rodgers as well. Also the paper of Migliorini 2012 is relevant here.*

25

**Answer:**

The references have been updated.

10. *Page 3, 129: "Both are based" It is not so clear what "both" refers to: the two studies, or SOFRID and MOCAGE.*

**Answer:**

30 We refer to SOFRID and MOCAGE DA system, the sentence has been corrected.

11. *Page 4, Section 2.1: METOP also has the GOME2 instrument. Has the synergy IASI-GOME2 been considered? Why the choice to use MLS?*

**Answer:**

MLS retrievals are very accurate and provide vertically resolved information that are inaccessible to UV sounders like GOME2. We used MLS to ensure an accurate stratospheric profile and evaluate the impact on IASI TIR assimilation, which was the focus of the study. The assimilation of GOME2 L2 profiles requires some particular care for correcting observation biases (Van Peet et al., 2018) and was not considered for this study. However, we agree with the reviewer's about the interest of performing IASI and GOME2 joint assimilation in future. We included this perspective in the conclusions of the revised manuscript (page 20, lines 1-2).

12. *Page 5, l4: "increased biases": what does "increased" refer to?*

**Answer:**

The word increased was removed.

13. *Page 5, l10: "LA" ?*

**Answer:**

LA stand for Laboratoire d'Aérodynamique, it has been replaced by B. Barret.

14. *Page 7, l11: "ECMWF NWP model" Please replace the word "model" by e.g. "NWP model and assimilation system".*

**Answer:**

Done

15. *Page 7, l19: The RTTOV versions for the L1 and L2 experiments are different, see table 1. Can the authors be sure that this does not significantly influence the results/conclusions?*

**Answer:**

The RTTOV version is now the same for both L1a and L2a and the revised manuscript has been updated based on new results. See also reply n 1 to the first reviewer.

16. *Page 7, l29: "... and was extended ..."*

**Answer:**

Correction included.

17. *Page 8, l19: "we assimilate here directly the full L2 profiles (43 levels)". Migliorini wrote a paper (2007) to discuss an efficient interface between L2 retrievals and data assimilation which is relevant in this context. Because the DOF is quite low, this implies that a lot of noise (43-DOF) is presented to the assimilation when all 43 levels are included. In principle*

*I agree that this avoids any loss of information, but in practice I wonder if the full information may introduce numerical issues (randomness) in the system, especially when this is combined with vertical interpolations? Please comment.*

**Answer:**

We agree with the reviewer about the pertinence of assimilating transformed SOFRID retrievals instead of the full profiles. This would reduce the cost of the L2 assimilation. However, we remind that in this study we used the full L2 error covariance matrices for the assimilation. Hence, the intrinsic noise of each observation level is somehow dampened within the computation of the cost function and its gradient. Source of randomness could result from inaccurate inversion of the observations error covariance matrices. As a matter of precaution, retrievals with inaccurate inverse were already excluded from the assimilation, but they represented less than 0.5% of all the available retrievals (before cloud filtering). Finally, the minimization always showed expected convergence behavior and we did not experience any particular randomness that could be related to numerical issues: repeating the same simulation twice gave same results within the precision of the output format (32 bit floating point). We added a sentence and the appropriate references in the revised manuscript to mention the possibility of using transformed retrievals (page 10, lines 8-11).

18. *Page 8, l22: "The steps for the computation of modeled radiances are equal to the profiles ones until the vertical interpolation." Please reformulate.*

**Answer:**

The sentence has been reformulated.

19. *Page 8, l27: "climatological profile" -> "climatological profiles"*

**Answer:**

Done.

20. *Page 8, l29: "as it is done within SOFRID retrieval scheme" please reformulate*

**Answer:**

Done.

21. *Page 8, l29: Does this mean that the SST is treated differently in the L1 vs L2 assimilation experiments?*

**Answer:**

No. Since SOFRID is a 1D-Var retrieval it does not propagate information to further retrievals as well, it also does not include any SST spatial error covariance. We better underlined the similarities between the two approaches in the revised text (page 10, lines 24-25).

22. *Page 9, l8: "initialized on 1st June 2010"; replace by "initialized on 1 June 2010"*

**Answer:**

Done.

23. Page 9, l11: "a diagonal matrix (i.e. with no inter-channel correlation) is used". Is the same diagonal matrix used in the retrievals that produce the L2 dataset?

**Answer:**

Yes. It is specified in the sentence before.

5 24. Page 9, bottom to p10, top: I got a bit lost with the numbers provided for the background standard deviation, also in comparison with Fig. 1. I understand that a background standard deviation during assimilation is often smaller than the std of a free model run, but I do not manage to connect the numbers with e.g. Fig.1 in combination with Fig.3?! What is the motivation to go from 5% to 2% in the stratosphere, which seems like a big step and does not seem justified given Fig.1? Does this choice lead to very small stratospheric increments? What is the justification for a step between stratosphere and troposphere? The standard deviation should depend on the data assimilated. Normally these kind of numbers are optimised with e.g. a chi-square test.

**Answer:**

15 The intent of Fig. 1 in the original manuscript was not to provide quantitatively values for the background standard deviation but: i) to display the main features of the error profiles ii) provide the reference values for the following figures that compare different experiments (Fig. 3 and 6 of the original manuscript). The empirical choice of values reported at page 9 resulted from a large number of experiments and we address the reviewer to the reply n 4 to the 1st reviewer for additional arguments that support the standard deviation values used in the end. In the reply n 5 we also show some examples of stratospheric increments that remain significant in terms of O<sub>3</sub> concentration.

20 The justification of using a step between the stratosphere and the troposphere follows from the vertical features of the errors. The modeled profile is generally more accurate in the stratosphere, especially when MLS is also assimilated (see Fig. 12 of the replies to the 1st reviewer). We are aware of the fact that the background standard deviation depends on the assimilated observations. However, the objective of the study being to compare L1 and L2 assimilation, we did not want to introduce additional differences between the experiments due to different background error covariances. Hence, the most pragmatic option was to find a sort of compromise that fits reasonably well for all the presented experiments.

25 The chi-square test is a useful diagnostics in DA but we did not consider it appropriate in our study for the following reasons: i) we use a very simplified observation error matrix and optimizing only the background error but keeping R fixed does not seem relevant ii) it is generally not possible to keep an optimum chi-square when using the same B but changing the assimilated instruments.

30 We included elements from these replies in the revised manuscript (page 12 and top of page 13) to better explain the reasoning behind the choices for B.

25. Page 10, l15: One would expect that features in the boundary layer, and, to a lesser extent, the free troposphere show vertical correlations because of e.g. vertical mixing and convection. This in contrast to the stratosphere.

**Answer:**

We agree in principle with the reviewer, and we did test a configuration with larger vertical correlations in the troposphere (1.5 model levels) than in the stratosphere (0.5 model levels), but results were not significantly better. We updated the text to include this element (page 12, lines 23-25, page 13, lines 1-2).

26. Page 10, first part: *I think the B matrix discussion can be shortened somewhat, because optimising it is not so important for the topic of the paper.*

**Answer:**

We removed some sentences corresponding to the settings employed in previous studies since they were not strictly necessary.

27. Page 11, l5: *"are in generally ", remove "in"*

**Answer:**

Done.

28. Page 11, l7: *"are found in correspondence of tropical latitudes". Please reformulate.*

**Answer:**

Done.

29. Page 11, l14: *"equivalence between L1 and L2 assimilation is not verified for O3". I suggest to explicitly add "for O3 retrievals in the thermal infrared".*

**Answer:**

Done.

30. Page 12, l2: *"The assimilation increases the RMSE of the tropospheric profile at northern latitudes (60N-90N)." I guess you mean in the range 350-1000 hPa.*

**Answer:**

The range has been added in parenthesis.

31. Page 12, l8: *"the other way round". Replace by "around".*

**Answer:**

Done.

32. Page 12, l17: *"Hence, we expect a stronger impact of the prior in the retrieval results,". I do not understand this. It means that the DOF is smaller, which is clearly observed at altitudes around 200hPa, where the improvement with IASI data is much more limited in the SH. But a-priori plays only a role through non-linear effects. Why would these non-linear effects be larger in the SH?*

**Answer:**

The reviewer's comment was very pertinent: our conclusion was not supported by the data (Fig. 1) but was a wrong interpretation of the original results (see reply n 1 to the 1st reviewer): the new experiments show indeed similar results also in the SH mid-latitudes. The discussion has been revised according to the new results.

- 5 33. Page 12, l27: *"The only exceptions are a lower RMSE degradation at 50 hPa". Should we believe the sondes or MLS here? How many sonde launches are included, and confirm the 60 hPa bias?*

**Answer:**

10 The number of radiosoundings has been reported in the revised manuscript, and we believe that higher confidence should be given to the MLS validation, especially with respect to standard deviation values. This aspect has been better highlighted in the revised manuscript (page 12, line 10 and page 16, lines 10-12).

34. Page 12, l32: *"total computing time is 3.9 CPU hours". Is this on a single core/node ??*

**Answer:**

15 The simulations have been performed on one Xeon E5-2680 node with 24 cores. The values given in hours are expressed in CPU time, which depends on the CPU type / frequency and give an approximate idea of the relative computational cost of L1a versus L2a. The run time (or elapsed time), given in minutes, depends on the parallel implementation and the number of cores/nodes used for the simulations. We replaced "total computing time" by "total CPU time" to avoid confusion.

- 20 35. Page 13, Fig.5: *The figure seems to prove that the analysis of MLS and of IASI are more consistent in the case of L1, while the L2 plot indicates biases between the instruments, especially in the tropics. This could be discussed a bit more explicitly.*

**Answer:**

Following the comment n 6 of the 1st reviewer, we replaced Fig. 5 with the MLS+L1a - MLS+L2a averages. The discussion has been revised accordingly.

- 25 36. Page 14, l16: *"mixed elsewhere"? Do you mean to say "mixed results are obtained elsewhere"?*

**Answer:**

The sentence has been changed.

37. Page 14, l22: *"which are differences" please correct the English.*

**Answer:**

The phrase has been corrected.

38. Page 14, l23: "reanalyses". I suggest to broaden this to e.g. "analyses and reanalyses".

**Answer:**

Done.

39. Page 14, l24: "between the L2 retrieval and the assimilation algorithm ". I suggest to change to " between the L2 retrieval and the L1 observation operator" or something like that

**Answer:**

Since we also extended the control vector of the assimilation, we rephrased with: "between the L2 retrieval and the L1 assimilation".

40. Page 14, l24: "using the same RTM". But the version of the RTM is different ?!

**Answer:**

The version of the RTM is now the same in the revised manuscript.

41. Page 14, l28: "between each other". I suggest "against each other".

**Answer:**

Corrected.

42. Page 14, l30: "Main findings suggest". I suggest "The results suggest ..."

**Answer:**

Corrected.

43. Page 15, l6: "We could imagine". I could as well, but is this a recommendation?

44. Page 15, l6: The non-linearity of the retrieval may be very different for different species and spectral ranges. Which ones would be candidates to show significant differences between L1 and L2?

45. Page 15, l9: I was wondering if we may expect positive synergies between IASI and GOME2? They are both on the same platform. Please discuss.

**Answer:**

This paragraph groups the the answers to the above 3 comments.

The original text at page 15, lines 3-8 was replaced since it was not appropriate anymore with the new results (reply n 1 to the first reviewer). We don't have enough experience with other retrievals than O<sub>3</sub> to give detailed recommendations on which species and L2 product might be affected by similar issues. Preliminary analyses indicate that O<sub>3</sub> profile retrieval in the UV region might display similar behavior than in the TIR. However, the degree of non-linearity depends significantly on the retrieval's a-priori: a case-by-case analysis would be needed in this sense. We included the perspective

of GOME2 assimilation in the revised manuscript and recommended to analyze potential dependence of the results to the a-priori (page 19, line 23).

46. Page 15, 115: "*Level 2 products can be aggregated*". This useful remark could be phrased more generally by referring to "*Use of the Information Content in Satellite Measurements for an Efficient Interface to Data Assimilation*" by Migliorini et al, 2007. Through L2 the number of useful observations presented to the assimilation may be optimised (to ultimately match the DOF).

**Answer:**

The methodology of Migliorini et al. (2008) is now referenced and briefly discussed in Sec. 3.3 (reply n 17). At page 15, line 15 we were specifically addressing models that does not cover the full atmosphere and the case of vertical selection/aggregation of measurements based on user needs. To our understanding, the method proposed by Migliorini et al. (2008) does not seem to be adapted this type of needs because it compresses the full retrieval's information.

## References

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