author comments on the manuscript "Vertical information of CO from TROPOMI total column measurements in context of the CAMS-IFS data assimilation scheme", reviewer 2

We would like to thank the reviewer for the constructive comments that aided us to improve our manuscript. In this document we provide our replies to the reviewer's comments. The original comments made by the reviewer are numbered and typeset in italic and bold face font. Following every comment, we give our reply. Here line numbers, page numbers and figure numbers refer to the original version of the manuscript, if not stated differently. Additionally, the revised version of the manuscript is added.

1 Major comments

1. ***Assumptions on formulating Equation (2) that relates CO profile and column The matrix A is the total column averaging kernel from TROPOMI CO column retrieval. As I understand it:***
x_{hat}–$x0 = A * (x - x0) + e$
where "x_{hat}" is the retrieved CO profile (its integration is the retrieved total column "c"); "x0" is the a priori in the retrieval algorithm; "x" is the "truth"; "e" is the error term. Then,
$x_{hat} + (A - I) * x0 = A * x + e$
Since the a priori "x0" or "(A-I)" is not zeros in the TROPOMI column retrieval algorithm, this term cannot be omitted. I would like to know the theoretical basis and assumptions made on formulating equation (2), which is the key equation for the profile retrieval method.
adjusted

We change the equation and description P5L120 from:

"So, we obtain the linear relation between the observed columns c and the profile x ,

$$c = \mathbf{A}x + e \tag{1}$$

with the Matrix $\mathbf{A} = (a_{ij}) = (a_i)$, with i =1...m and j=1...n.."
to

"So, we obtain the linear relation between the observed columns c and the profile x ,

$$c = \mathbf{A}x + (\mathbf{I} - \mathbf{A})x_{apr} + e \tag{2}$$

with the Matrix $\mathbf{A} = (a_{ij}) = (a_i)$, with i=1...m and j=1...n and the a priori profile x_{apr} based on TM5. For profile scaling retrievals as used for the TROPOMI CO data the term $(\mathbf{I} - \mathbf{A})x_{apr} = 0$ (Borsdorff et al., 2014). Hence, we can reduce the equation to

$$c = \mathbf{A}x + e \tag{3}$$

"

2. ***(2) Effectiveness of the a posteriori profile retrieval method should be evaluated using simulation spectra The way to infer the profile from column and column AK is interesting. However, simulation study (so called OSSE) should be carries out to make sure the method works properly. In this way to make sure the retrieval results are not significantly biased, and to quantify the error budget from the a posteriori profile retrieval algorithm***
not adjusted

Our approach is an application of the standard inversion theory for profile inversion that is well established, tested, and applied in scientific community for decades (please the see the publications by e.g. Borsdorff et al. (2014), Phillips (1962), Rodgers and Connor (2003), Twomey (1963)). Our idea of combining the total column averaging kernels is also based on the theory of the standard linear inversion. Of course we tested our numerical implementation but we think that a OSSE study would create overhead in our manuscript and would not add anything to the already established inversion theory. The aim of our manuscript is to apply the theory to show that TROPOMI can improve CAMS-IFS. That is a different objective than validating the inversion theory.

2 Specific comments

1. ***Line 9: change "individual ... retrievals"***
   adjusted We replace "individual" by "an ensemble of"

2. ***Line 11: remove "the" before date.***
   adjusted We applied that for all dates in the whole document.

3. ***Line 38: rephrase "are supplied by the data product"***
   adjusted We changed the sentence P2L38 form:
   "...are supplied the data product."to
   "are supplied with the data product."

4. ***Line 50: comma before "respectively"***
   adjusted

5. ***Line 81: correct the citation format***
   adjusted

6. ***Line 125: left hand side of Equation (3) should be the cost function value, not x_{ret}. Equation (3): Which is used for x_{apr} in the retrieval algorithm? Is it TM5 simulations? Please add that in the paragraph.***
   adjusted Please see our answer to the first comment of the referee. We updated the manuscript accordingly and defined x_{apr} and referenced to TM5. We add the following sentence at page P5L26:
   "Here the function $\min_x$ is providing the profile that minimizes the Tikhonov cost function."

7. ***Line 138: in better agreement with TROPOMI CO columns retrieved using profile scaling?***
   adjusted We add the following sentence at P6L152: "This special type of a profile retrieval is becoming a profile scaling retrieval when the regularization parameter $\lambda \to \infty$."

8. ***Results section: I would suggest to separate this one big section into 3 parts based on the three different cases.***
   adjusted

   We divided the results section 4 in three parts:
   4.1 Rabbit Foot Fire in Idaho
   4.2 Pollution transport from Siberia to Canada
   4.3 Seasonal biomass burning in the Amazon

9. ***Line 158: CAMS-IFS assimilates IASI and MOPITT only. The reason the pollution pattern does not show up in the simulation may be because both satellite data failed to capture the anomalies. Please see the images of IASI CO below Very likely due to clouds over the fire plume (seen from the MODIS image on the same day), IASI did not make the retrieval. Therefore, it is not reflected in the CAMS-IFS. Adding this background information may help readers to understand the discrepancy between TROPOMI and CAMS-IFS.***
   adjusted

   We change the sentence at P6L15 from:
   "This can be either due to missing emissions of the fire in the model or a time delay of the emissions used in the forecast run of the model. In both cases the assimilation of TROPOMI data in CAMS-IFS can help to improve the issue. " to
   " This event was not captured by the MOPITT or IASI satellite measurements most probably caused by clouds over the location of the biomass burning. Hence, the prediction of CAMS-IFS for this case fully dependents on the assumed fire emissions in the model. Consequently, a reason for the missing plume in the CAMS-IFS model could be missing emissions or the one day time delay of fire emissions in the CAMS-IFS forecast run. For all cases the assimilation of TROPOMI data in CAMS-IFS can help to improve the issue. "

10. ***Line 159: "This can be either due to missing emissions of the fire in the model or a time delay of the emissions used in the forecast run of the model." You can easily check that by looking into the temporal changes of CO simulations in CAMS-IFS. Or, as I point out above, this is because the IASI data feeded into CAMS-IFS failed to capture the high CO plume.***
    adjusted

    Please see previous comment.

11. ***Line 184, comma before "respectively"***
adjusted

12. ***Figure 1: Do the different colors have meaning? The column averaging kernels differ largely, what are the primary cause? There is an outlier in light blue, which has AK values close to 1.0 for all layers, representing a very ideal case. Why does this one look so peculiar? Also, please rewrite the x- axis label.***
adjusted The outlier is a typical clear-sky total column averaging kernel hat shows full sensitivity through the atmosphere.

We change the figure caption from:
"Total column averaging kernels of the TROPOMI CO retrieval for different satellite ground pixels selected over the Amazon during the burning season (1 August 2019 to 15 August 2019)"

to "Total column averaging kernels of the TROPOMI CO retrieval for different satellite ground pixels (color coded) selected over the Amazon within the burning season (1 August 2019 to 15 August 2019) in unitless representation [1]. Most of the retrievals are cloud contaminated."

13. ***Figure 2: please correct the subscript formats for x-axis and y-axis labels***
adjusted

14. ***Figure 3: Please explain the difference of the physical meaning of AK columns and rows.***
adjusted We changed the caption from:
" Averaging kernel of the posteriori profile retrieval for CO over the Amazon during the burning season (1 August 2019 to 15 August 2019). The left panel (a) shows the rows and the right panel (b) the columns of the averaging kernel matrix. The corresponding altitudes are giving in the legend. "to
" Averaging kernel of the a posteriori profile retrieval for CO over the Amazon (1 August 2019 to 15 August 2019) within the burning season in unitless representation [1]. The left panel (a) shows the rows and the right panel (b) the columns of the averaging kernel matrix. The rows indicate how one level of the retrieved profile is a smoothed version of all level from the true profile while the columns show how one level of the true profile will affect all level of the retrieved profile. Altitudes are giving in the legend. "

15. ***Figure 7-9: Is a way to add error bars for the CO profile retrievals to show if the difference is significant or not?***
not adjusted

We can only propagate the noise error of the total column retrievals on the profile. However, due to the large amount of combined retrieval this error bars are becoming to small to be significant. To get an realistic error estimation we would need the spatial and temporal correlation of the errors on the atmospheric input data which is not available. However, such a error analysis should be better done within an assimilation scheme like CAMS-IFS.

3 Additional changes

1. ***A new co-author is added to the manuscript***
adjusted
We added Kyle J. Zarzana as an new co-author and removed the reference to him from the acknowledgements.

References

Borsdorff, T., Hasekamp, O. P., Wassmann, A., and Landgraf, J.: Insights into Tikhonov regularization: application to trace gas column retrieval and the efficient calculation of total column averaging kernels, Atmospheric Measurement Techniques, 7, 523–535, https://doi.org/10.5194/amt-7-523-2014, URL `https://doi.org/10.5194/amt-7-523-2014`, 2014.

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