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Comment on amt-2022-315

Anonymous Referee #1

Referee comment on "Vertical information of CO from TROPOMI total column measurements in context of the CAMS-IFS data assimilation scheme" by Tobias Borsdorff et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2022-315-RC1, 2022

"Vertical information of CO from TROPOMI total column measurements in context of the CAMS-IFS data assimilation scheme" by Borsdorff, Campos, Kille, Volkamer, and Landgraf.

The manuscript describes a method to derive a posteriori CO vertical profiles using TROPOMI CO vertical column retrievals and their associated total column averaging kernels (AK). The a posteriori profiles are then compared with respect to airborne CO vertical profiles (Rabbit Foot Fire) and assimilation results, both vertical profiles and total column values, obtained with CAMS-IFS (Rabbit Foot Fire, Siberian fires, Amazon fires). CAMS-IFS assimilates vertical CO profiles (and their corresponding AK too? Unclear from the manuscript) from MOPITT and IASI. TROPOMI total CO columns and their AK will also be assimilated by CAMS-IFS starting in Q2/2023. TROPOMI will be a valuable contribution to CAMS-IFS assimilation results because of its high spatial resolution (higher than MOPITT's and IASI's) and daily coverage (better than MOPITT's). The importance of TROPOMI's contribution to the CAMS-IFS assimilation in terms of vertical sensitivity to CO would be more clear if additional comparisons had been presented: comparisons to airborne and satellite vertical profiles, as well as comparisons involving more than one TROPOMI a posteriori profile per study case.

This is important work and deserves publication once the issues listed are properly addressed. We identify the following two main issues:

1. In the Rabbit Foot Fire case, one vertical CO profile retrieved from TROPOMI column measurements using the a posteriori profile retrieval method is compared to one collocated airborne vertical profile acquired during the BB-Flux campaign. In each of the other two study cases (Siberia and Amazon fires), one vertical CO profile retrieved from TROPOMI columns is compared to one CAMS-IFS assimilation profile, rather than to actual CO measurements or retrievals. If collocated airborne vertical profiles were unavailable (please discuss in the manuscript if that was the case), such comparison could have been performed using collocated MOPITT and/or IASI vertical profiles. Comparisons to actual measurements/retrievals would be more direct than (and complementary to) comparisons

to assimilation results. Please, either compare vertical profiles from TROPOMI and these other two datasets in the manuscript or justify why such comparisons are not performed.

2. In each of the three study sites (Rabbit Foot Fire, Siberia and Amazon fires) the performance of the a posteriori retrieval method is discussed based on a single TROPOMI vertical profile (as well as on one CAMS-IFS and one TM5 profile) per site. To make for a stronger case, please provide multiple examples per site; that would show better the significance of these results.

Minor issues concerning style/language:

Line 6: "VCD" not used again, please consider removing, for simplicity.

9, 115, 123, 216: "an a posteriori"

14: for context, what are the horizontal dimensions of the plume?

17-18: "CAMS-IFS underestimates the enhanced CO vertical column densities sensed by TROPOMI within the plume by more than 100 ppb". What do MOPITT and IASI show regarding total column values? Would aerosols affect differently the SWIR (TROPOMI) and the TIR (MOPITT, IASI, and, thus, CAMS-IFS results)? Please address in the main body of the manuscript.

18: "During the burning season (1 - 15 August 2019)". Wording implies that the burning season lasts only those 15 days.

23: "carbon monoxide (CO)"

24: "Its only sink is the oxidation reaction with the hydroxyl radical". OH is the main sink of CO, but not the only one: soil is another important CO sink (e.g., Cordero et al., 2019, Stein et al., 2014).

28: please place "e..g.," inside the parenthesis.

32: “spatial resolution of 5.5 × 7 km 2 (7 × 7 km 2 before 6 August 2019)” already in Abstract. To avoid repetitions, please consider removing “(7× 7 km 2 before August 2019)” from Abstract.

33-34: “and the shortwave infrared (SWIR, 2305-2385 nm)”

34, 69, 70: Consider using “SWIR” instead of “shortwave infrared”

38: “that are supplied with the data product”

40: should “and is released for public usage” be “; thus, the TROPOMI CO dataset was released for public usage”?

42: consider rewording to “The TROPOMI CO data set was compared early in the mission with”

46: for simplicity, consider rewording to “Currently, total column CO retrievals from MOPITT (Measurement of Pollution in the Troposphere instrument) and IASI (Infrared Atmospheric Sounding Interferometer) are routinely assimilated (Inness et al., 2015). The spatial resolution at nadir of these datasets is near 22 x 22 km2 and 12 x 12 km2, respectively.”

53: TIR measurements, which are sensitive to the vertical distribution of CO, are most sensitive in the mid troposphere. Are NIR measurements sensitive to the vertical distribution of CO at all?

59: for simplicity, please consider rewording to “varies for clear and cloudy conditions and with observation geometry”.

60: Please justify: “Hence the TROPOMI CO observations effectively probe CO in different altitudes.”

61: “we implemented an a posteriori profile retrieval method”

63: what were the collocation criteria?

64: please reword to “collocated CAMS-IFS simulations that do not assimilate”

65, 81, 101, 102, 137, 139, 154, 166, 169, 175, 190, 194, 197, 211, 212, 226, as well as captions of Fig. 2 (x2), 3, 4, 5, 6, 7, 8, 9: “a posteriori” rather than “posteriori”

Similarly, “priori” should be “a priori” in, for example, lines 78, 138, 165, 173, 211, 239, and caption of Fig. 7. Alternatively, please use “prior” instead of “a priori”.

66: “demonstrates the approach using three CO pollution cases”

69: the first sentence in the paragraph repeats information already provided in Section 1.

79: please define “low cloud” in mofre detail.

83: please simplify to “with the simulated CAMS-IFS CO fields.” CAMS-IFS had been defined earlier.

86-87: “The aim of CAMS-IFS is to forecast the atmospheric composition in near real-time up to five days ahead provided 6-hourly with a spatial resolution of approximately 40 × 40 km 2.” already in Section 1.

87-90: ”CO total column measurements from the Measurement of Pollution in the Troposphere (MOPITT) instrument and the Atmospheric Sounding Interferometer (IASI) are assimilated routinely. ECMWF plans to assimilate the TROPOMI CO columns and their vertical sensitivities (total column averaging kernels) with CAMS-IFS as well.” already in Section 1.

92-94: “The TROPOMI CO data is already monitored since 2018 within the CAMS-IFS

system and the final assimilation will be activated in the next operational upgrade (CY48R1) scheduled for Q2/2023 (Inness et al., 2022).” already in Section 1.

98: is “ε” provided with each TROPOMI retrievals? how is “ε” calculated?

104-105: please reword “carbon monoxide” to “CO”.

105: please provide precision and accuracy of the airborne measurements. Only one airborne CO profile is shown (Fig. 7a), were any other relevant CO profiles acquired? Having all results and interpretations for this study case based on a single profile is not very persuasive.

106: “an optically thick pollution plume”

107: “This date”

108: “These in-situ measurements are in an excellent spatial and temporal overlap with TROPOMI measurements” Please provide collocation details: how many hours and km apart are they?

109: for clarity and simplicity, please consider rewording “They validated TROPOMI CO retrievals […] of the retrieved CO profile from the TROPOMI data.”. Please define FLEXPART.

115-152: This section may be at times difficult to follow for those who are new to this retrieval process. Please define explicitly each new term as it is introduced and provide sufficient background for all readers to gain a basic understanding of the reasoning behind the a posteriori retrieval method.

115: how many layers? At what altitudes/P levels? What criteria were used to select their number and vertical location?

116: would it be “using TROPOMI total column data with different vertical sensitivities.”?

116: The text states that the a posteriori profile is “representative for a selected region and time range”. What criteria (box size, location) are used to group those TROPOMI retrievals?

117: How is “e” calculated?

121: please clarify (a_{ij}) = (a_i). Does “i” refers to retrieval and “j” to vertical layer?

From line 97: a_{col}=total column averaging kernel for the TROPOMI total column retrievals. And from line 121: a_i=total column averaging kernel. Please clarify what is the difference between both.

129: how is “λ” calculated?

137-141: Ideally, total column derived from the a posteriori TROPOMI vertical profiles should be equal to the (averaged?) retrieved TROPOMI total columns; please explain why is that not the case. Also, retrieved TROPOMI total column should differ from total column calculated from TN5 profiles, at least in polluted cases; otherwise, the TROPOMI retrieval would be just a duplicate of its a priori. This paragraph states that the a posteriori profile (at least for the one profile in the Amazon – results from more profiles would make for a much stronger case) is closer to the TM5 profile than the TROPOMI retrievals were; that seems to indicate that actual information in the TROPOMI total column from the “standard” retrieval got lost in the a posteriori profile retrieval. Please clarify and discuss in the Conclusions section. Are similar discussions provided for the Siberia and Amazon cases?

154: The manuscript would be much stronger if TROPOMI a posteriori vertical profiles were compared with respect to other measurements/retrievals, from MOPITT and IASI if airborne profiles are not available.

154: “We applied the a posteriori profile retrieval approach to three different cases.”

156: “and by that” is unclear, please reword.

158: “near Boise, Idaho”. For context, please discuss horizontal size of plume and place in the context of TROPOMI, MOPITT, IASI spatial resolution and coverage. Any profiles from MOPITT and IASI sampling the plume?

162: How was bias calculated? is TROPOMI higher or lower than CAMS-IFS?

163: “The TM5 CO field is a monthly average with a coarse spatial resolution of 3 â□¦ x 2 â□¦”. However, panel 4.c shows color variations in the pixels represented, which appear to be the same size as the pixels in panels a and b, and much smaller than 3x2 degrees. Please clarify.

165: “It is worth mentioning that TM5 serves as the priori for the TROPOMI CO retrieval”. Please consider moving to “Datasets”

165; 206; and captions of Fig. 4, 5, and 6: please consider rewording “black dashed square” to “black dashed box”, since those figures are not square.

168: Fig. 7 is introduced in the text before Fig. 5 and 6.

173: “when representing the retrieved profile of TROPOMI relative to its TM5 priori” Does that mean that the posteriori TROPOMI profile was divided by the TM5 profile?

176: please add a smoothed version of the BB-Flux profile to Fig. 7a for a more direct comparison to the a posteriori TROPOMI profile. Unclear how the BB-Flux profile shown in 7b was processed.

175-176: “We also smoothed […] TROPOMI measurements” is the smoothed BB-Flux profile shown somewhere?

179: “Arctic Ocean”

179: should it be “Figure 5 (d)” ?

182: consider rewording “surprisingly good agreement” to “remarkably good agreement” or similar.

183-184: “with a bias of […] respectively”. Are those stats for pixels inside the box only or for the entire region mapped? How was bias calculated, is TROPOMI higher or lower than CAMS?

185: what's the time of day of the CAMS-IFS maps? How does it compare to TROPOMI's?

186: "a time mismatch between the real emissions and the ones assumed in the forecast run of CAMS-IFS" Please clarify the cause and magnitude of that possible mismatch.

192: maybe "shows a similar shape", since they peak at different altitudes and their overall shapes differ quite a bit.

199: Fig. 6 is introduced after Fig. 8.

202-203: "with a bias […] during the biomass burning season". Are those stats for pixels inside the box only or for the entire region mapped? How was bias calculated, i.e., is TROPOMI higher or lower than CAMS?

205, 208: "a posteriori"

210: "agree well and represent"

214: for consistency, please quantify bias and R in this case too for a posteriori TROPOMI versus CAMS-IFS.

218: collocation criteria? Please provide details early on, in the Datasets section, for example.

219: please correct to "simulations that do not assimilate"

223: "no pollution plume is present in the model data." Is that because MOPITT and TROPOMI did not capture the plume? Is the plume too small for their spatial resolution? Please explain.

225-226: "This even […] posteriori retrieval" Please clarify why is this case challenging.

229: “all days” or “both days”?

231-232: please clarify “because the emissions seem to be higher for the next day.”

243: “to some extent”

244: “due to the fact”, “cloudy conditions”

247: consider rewording to “not only clear-sky measurements are valuable” or similar.

Fig. 1: axis label “a[1]” unclear, does it mean “TROPOMI total column averaging kernel [unitless]”?

Fig. 2: Are the axis labels correct (please explain) or are the ”_{2}” formatting commands? Please explain what are “Kx” and “y”. Also, please correct “to find the the regularization” Caption: is “α” explained elsewhere?

Fig. 3 caption: 1-15 Aug 2019 is probably not the entire burning season; please reword. Also, reword to “altitudes are given in the legend.” Please explain what do the AK rows mean. And the AK columns? Please clarify “[1]” in horizontal axes; should they say “… of A [unitless]”?

Fig. 4 caption: for clarity, please consider rewording to, for example “CO total columns for 12 August 2018 from TROPOMI orbit 4305 (a), the CAMS-IFS model (b), and the TM5 model (c). TROPOMI measurements show elevated CO from the Rabbit Foot Fire near Boise, Idaho which was not captured by either of the two models. The black dashed box shows the region analyzed in our a posteriori profile retrieval analysis.”

Fig. 4 caption: add information regarding the spatial resolution in each case. Same for Fig. 6. Please clarify in the main text if a single a posteriori TROPOMI profile was obtained from data in the ~2x3 degree (~222x333 km^2) box shown in panel 4a. What criteria were used to select the box?

The following applies to analyses summarized in Fig. 4, 5, and 6: How many TROPOMI retrievals went into calculating the one a posteriori vertical profile? Were all the TROPOMI retrievals used, or were they filtered (and how)?

The following applies to Fig. 4, 5, and 6: The text states that the spatial resolution of CAMS-IFS is 40 x 40 km^2/pixel and that of TM5 is 3 x 2 degrees/pixel (i.e., ~ 333 x 222 km^2/pixel). However, in these maps the pixel size of both CAMS-IFS and TM5 appear to be much smaller that that, and about the same size as TROPOMI's (~ 5.5 × 7 km^2). Please clarify if the maps have been supersampled or similar; maps with the actual spatial resolution of each dataset would be best.

Fig. 6: Please clarify in the main text if a single a posteriori TROPOMI profile was obtained from data in the ~10x5 degree (~1110x555 km^2) box shown in panel 6d. What criteria were used to select the box?

Fig. 5: Similarly: please clarify in the main text if a single a posteriori TROPOMI profile was obtained from data in the ~50x15 degree (~5600x1700 km^2) box shown in panel 5d. What criteria were used to select the box?

Fig. 7: The in situ BBFlux profile sampled from ~4.5 km to ~ 0 km altitude. However, Fig. 7b shows a transformed BBFlux profile getting all the way up to ~15 km altitude. How was that accomplished?

Fig. 8 caption: "enhanced TROPOMI CO column measurements", please explain what does "enhanced" mean here.