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Comment on amt-2022-241

Anonymous Referee #1

Referee comment on "Exploring bias in the OCO-3 snapshot area mapping mode via geometry, surface, and aerosol effects" by Emily Bell et al., Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2022-241-RC1, 2022

Manuscript “Exploring bias in OCO-3 Snapshot Area Mapping mode via geometry, surface, and aerosol effects” submitted for publication in Atmos. Meas. Tech. (AMT) by Bell et al. is addressing an important topic appropriate for AMT, covers new and interesting aspects related to the space-based retrieval of CO2 and is very well written. I therefore recommend publication after the (mostly minor) aspects listed below have been carefully considered by the authors when generating the revised version of this paper.

General comments:

In the future several satellites will be launched aiming at monitoring CO2 emissions from localized CO2 emission sources such as power plants and cities using “atmospheric CO2 imaging” combined with inverse modelling (as explained in Bell et al.). OCO-3 on the International Space Station (ISS) is the first space-based instrument that acquires CO2 images thanks to its Snapshot Area Mapping (SAM) observation mode. A careful analysis of the OCO-3 SAM XCO2 data product is therefore not only important to maximize the scientific output of this mission but also to learn for and ultimately improve future CO2 monitoring satellite missions. The authors present detailed results from simulations and analysis of real data addressing the important issue of XCO2 retrieval biases due to uncertainties related to observation and solar geometry, surface reflectivity, aerosols, etc.

The authors focus on a few cases (scenes) which are assumed to be representative. They highlight potential limitation to be addressed via future work. I consider this approach acceptable. However, I am missing some relevant references which I recommend to add (see also below). For example, I recommend to add Reuter et al., 2019, when citing Nassar et al., 2017, as this is another study where OCO-2 data have been used to obtain information on power plant CO2 emissions. I also recommend to add references to the future missions listed in the paper (MicroCARB, GeoCarb, GOSAT-GW, CO2M). In particular, Rusli et al., 2021, should be cited as their investigation on aerosol related XCO2 biases is relevant for this publication, which also highlights aerosol related issues.

Specific comments:

Page 2, line 25 following: Sentences "Since the launch of the Greenhouse gases Observing Satellite (GOSAT; Kuze et al., 2009; Yokota et al., 2009) in 2009, space-based instruments have been addressing the particular challenge of scale. In decades prior, the global carbon cycle was studied using a handful of highly localized ground measurements scattered across, mostly, the northern hemisphere land surface; …":

Strictly speaking this is not true. The first space-based instrument measuring XCO2 was SCIAMACHY on ENVISAT (Bovensmann et al., 1999), launched already in 2002, and SCIAMACHY XCO2 retrievals have been used to study the carbon cycle already before (e.g., Buchwitz et al., 2007; Schneising et al., 2008) but also after (e.g., Reuter et al., 2014; Schneising et al., 2014) the launch of GOSAT. This information needs to be added.

Please add more information and if possible also references on the "challenge of scale" aspect. What exactly is the challenge? Where has it been addressed?

Page 2, line 50: Sentence "… producing a data-dense, spatially coherent map of XCO2.":

As the maps shown in the paper indicate that the OCO-3 SAM XCO2 product suffers from significant biases I would conclude that the goal of generating "spatially coherent map of XCO2" has not yet been achieved. I recommend to write "aims to produce" (or equivalent) instead of "producing".

Page 2, lines 56-57, sentence "Point source signals are difficult to quantify because the XCO2 enhancement is often two orders of magnitude smaller than the background concentration":

The difficulty does not arise from the fact that the enhancement is two orders of magnitude smaller than the background concentration, but from the fact that the instrument noise is about the same order of magnitude as the enhancement.

Figure 1: According to the figure caption the left figure shows "a power plant plume". Visible in wind direction are two areas of elevated XCO2 (instead of a single plume area). Is it possible to comment on this? Is this supposed to be a real feature or a bias related artefact? Interestingly the TROPOMI NO2 figure on the right shows something similar (despite the time difference).

Page 7, equation (1):

The interpretation of sb_ratio as "swath bias" assumes that the (real) CO_2 plume is negligible in terms of amplitude and/or area coverage, or? If yes, then I recommend to add this information.

Page 8, line 186 and following: The dP_abp filter seems quite relaxed as a 16 hPa surface pressure error corresponds roughly to 1.6% or 6 ppm for XCO_2. It is written that this is part of "a simple post-processing quality filter". In the previous paragraph it is written that ABP is part of the pre-processing. I find this confusing. Is the filter used for post-processing but computed already during A-band pre-processing? Is this a difference between the operational retrieval algorithm and the one used here? Please clarify. Is the pressure difference dP also computed using the retrieved state vector elements (if surface pressure is a state vector element) originating from the main (3-band L2FP algorithm) retrieval and if yes is this (L2FP) dP also used for quality filtering and bias correction? And if not, why not?

Page 8, line 205. Figure 5c is mentioned, but there is no figure 5c, because figures have no (a), (b) ,…, labels. The "f" in "figure" should be capitalized.

Page 11, section 5:

I understand that the retrieval algorithm/code as applied to the simulated XCO_2 data is exactly identical with the algorithm/code used to analyse the real OCO-3 data apart from different spectroscopic input data. Or are there any significant (other) differences (including pre- and post-processing)?

Figure 6 and related discussion (including Figures 10 and 15):

The simulated XCO_2 as shown in the top right panel shows a large discontinuity – a XCO_2 "jump" of several ppm between the "4 bottom left swaths" and the "4 top right swaths". It is concluded that: "We find that simulated spectra derived from simple aerosol scenes are successfully able to generate SB patterns similar - though not identical - to those in the operational vEarly data". Yes, but why? This is not clear for me and I find this very surprising. I would have expected a more smoothly varying bias assuming that neither the surface properties nor the aerosols show a corresponding jump. Is this assumption true for the simulations (I assume that maps of the relevant input parameters have been generated and investigated)? Which input parameter as used for the simulations shows a similar jump and can therefore explain the XCO_2 jump? If all input parameters vary smoothly than the result indicates that the retrieval algorithm seems very sensitive to small changes of certain input parameters as used for the radiative transfer simulations to generate the simulated spectra. In this case, for some reason, the retrieval responds with a jump from one state to another, which is a bit unexpected. I recommend to generate and inspect maps of relevant input parameters (in particular also viewing angles) which may explain the jump including parameters such as the relative azimuth angle between line-of-sight and sun direction which may also jump / change sign. In this context: I assume that the swaths are not parallel to the flight direction and the "4 bottom left swaths" are not on one side of the sub-satellite track and the "4 top right swaths" are not on the other side, or? In any case please add information on how the scans are performed in terms of timing (I assume that there is only a small time difference between the different swaths and that one swath after the other (from left to right or the other way around) is measured).

The results shown in the bottom right panel of Figure 6 are even more surprising as the between swath jumps are even less systematic also suggesting the issues may be related to certain angles (assuming that none of the other input parameters is spatially correlated with the swaths).

Figure 10 shows that the retrieved XCO2 (from the simulations) significantly "jumps" depending on the assumed aerosol type with more or less large XCO2 jumps within the scene. Again, this is surprising if surface and albedo properties are not spatially correlated with the XCO2 bias pattern.

Figure 15 shows that dP also "jumps", i.e., shows a spatial pattern correlated with the XCO2 bias. Is the dP shown in the bottom left panel computed with the operational ACOS ABP algorithm (using only the O2-A-band) or is it computed using output from the 3-band L2FP retrieval? It seems that the XCO2 jumps are strongly related to dP jumps (and therefore using dP for bias correction helps to reduce biases). As dP originates (entirely or mainly) from the O2-A-band then the question is if the origin of the XCO2 biases is related to the use of the O2 A-band (as part of the 3-band L2FP retrieval)? Can it be excluded that the use of the O2-A-band causes the presented XCO2 biases (in particular the XCO2 jumps)?

Page 19, line 405-406, sentences: "we surmise that the trend toward SB at higher albedos is not because SB is more likely to occur over bright scenes. In fact, stronger SB tends to occur at lower albedos" but "The SB is highest at lower albedos" (lines 398-399):

Which trend toward SB at higher albedos is this referring to?

Page 22, lines 468-469: "we first apply the more restrictive v10 sounding selection criteria to vEarly":

Do these selection criteria refer to the quality filter? Because right after that sentence: "We apply quality filtering and bias correction, narrow down to only SAMs with at least

500 soundings (N>500), and calculate our SB parameters from Equation 1. vEarly quality filtering is our custom | dP_abp | < 16 hPa filter, and v10 is filtered using the operational v10 quality flags. Figure 16 details the comparison". Which filter is used for vEarly? According to results apparently the custom | dP_abp | < 16 hPa filter.

Figure 16, caption: the histograms seem to be normalized. I would add this information. The abbreviation NSAM (in the figure) is not explained.

Page 23, line 481: "Bias correction alone reduces the frequency of v10 SB cases from 11.9 to 10.4%": These numbers do not match the NSB/NSAM shown in Fig. 16:

(vEarly) 378/2685 = 0.14

(v10) 202/1749 = 0.12

Do the percentages refer to something else? The 11.9% matches the numbers mentioned in page 8, lines 191-192. If this is the case, the total set of SAMs for the comparison is not the same.

Page 25, line 512: I recommend to add NO_2 after TROPOMI: TROPOMI NO_2 indicates …

Page 26, caption Figures 19 and 20: Please add info on which product is shows in which panel. Is the product shown in the middle the "Lite" product?

Page 26, line 530, sentence "… we observe a new geometry-related bias …": This sounds that it can be excluded that OCO-2 retrievals also suffer from this bias. As the OCO-3 data are similar as the OCO-2 data and also the retrieval algorithm is essentially the same I am not sure that this is really a new bias in the sense that only OCO-3 data suffer from it. Have similar issues (especially XCO_2 jumps) also been observed for OCO-2 (e.g., target mode observations)?

Page 26, line 532 following, sentence "… by calculating the ratio of swath-to-swath noise in the XCO_2 field to the …": This quantity is referred to as swath bias in the paper as it is a systematic error and not a random error, i.e., not noise. I recommend to replace "noise" by "scatter" or "standard deviation of the medians computed for each swath" or equivalent.

Page 27, line 535 following: Why are so many fossil targets suffering from swath bias? Can this be an artefact of the analysis as the computation of the indicator (see Eq. 1) assumes negligible plumes?

Page 27, line 561, sentence "Finally, we replicate our vEarly analysis using the updated version 10 dataset, and see vastly improved statistics. We find that improved quality filtering is the primary driver of this development, …": I guess that "vastly improved statistics" primarily refers to relative (percentage) performance (as filtering removes data) but not to absolute performance in terms of also more good data. Please extend this statement so that it is clear if also the absolute number of "good" retrievals is enhanced or not.

Typos etc.:

Figure 4: I recommend to harmonize the time information ("Jul." vs "July") in the figure caption.

Page 8, line 205: "of important" -> "of importance" (or equivalent)

Page 12, line 295: representative

Page 19, line 407: "aerosols and dark surfaces" ☐ "aerosols over dark surfaces"

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