

Authors' Response to Reviews of

Methane retrieval from MethaneAIR using the CO₂ Proxy Approach: A demonstration for the upcoming MethaneSAT mission

RC: *Reviewers' Comment*, AR: Authors' Response, □ Manuscript Text

1. Comprehension

RC: *The manuscript presents shortwave infrared methane measurements using MethaneAIR, an airborne demonstrator for the MethaneSAT satellite. The study focuses on retrieval performance and validation of the CO₂ proxy method for CH₄ retrieval, addressing instrumental challenges like ISRF drifts, and implementing bias correction techniques. It also validates MethaneAIR's measurements against ground-based data. The preprint aims to extrapolate its findings to anticipate the performance of the forthcoming MethaneSAT mission, particularly in terms of precision and detection limits for methane emissions. The study presents valuable and relevant research but necessitates revisions, particularly in the description of methodologies and structural organization, to ensure clarity and completeness before it is suitable for publication.*

We thank the reviewer for their time and helpful suggestions for the manuscript. Our responses to their comments are below.

2. General Comments

RC: *The manuscript's extrapolation of findings from MethaneAIR to MethaneSAT requires improvement, as it frequently lacks comprehensible detail on how this projection is methodologically executed (including the assumptions and limitations).*

AR: We have added a section (S2) to the supplement to address these issues. This includes performing a linear sensitivity analysis to estimate the measurement precision of MethaneSAT with what is currently known about the sensor (Section S2.1).

RC: *What types of errors can lower spatial resolution introduce, such as the omission of low-contrast pixels, among others?*

AR: Section S3 now includes additional details on potential issues caused by the lower spatial resolution of MethaneSAT. These include

- Cloud contamination (Section S2.3.1)
- Inhomogeneous illumination (Section S2.3.2)

- Sub-pixel CH₄ concentration gradients (Section S2.3.3)

In general we do not find significant differences in performance between the two sensors for the error sources considered.

RC: *The discussion about e.g. the 0.15% target precision for MethaneSAT and its relation to MethaneAIR's performance is limited and I can't clearly see how this extrapolation is methodologically done.*

AR: This was just based on the central limit theorem. By aggregating pixels the precision of the sample mean concentration ($\bar{\sigma}$) should follow

$$\bar{\sigma} = \frac{\sigma_0}{\sqrt{n}} \quad (1)$$

Where n is the number of pixels and σ_0 is the single-pixel precision. We have added a footnote to clarify how this was calculated.

RC: *A numerical analysis of the uncertainties associated with emission estimates would be desirable.*

We have updated the manuscript to include emissions uncertainties for the emissions estimates derived from the IME method. The methodology for these estimates is described in the manuscript cited in the paper (Chulakadaba et al., 2023).

RC: *Section 8 of the manuscript is relatively brief considering its title, suggesting a need for more extensive coverage and depth in its content.*

AR: We have expanded the MethaneSAT discussion, with links to the supplement for further information

Importantly, we find no strong dependence on surface reflectance in the MethaneAIR results. This was a key untested assumption in the early emissions inversions observing system simulation experiments that were used to inform the MethaneSAT instrument requirements (Benmergui, 2019). In those original experiments the assumed precision of MethaneSAT was 0.15% at $1 \times 1 \text{ km}^2$ resolution. In follow up experiments it was found that the satellite could meet its emission constraint goals with that precision at a scale of $5 \times 5 \text{ km}^2$. We expect MethaneSAT to have a similar per-pixel precision as MethaneAIR (35 ppb, Section S2.1). At these levels the 0.15% target precision will be achieved at a scale of $\sim 3 \times 3 \text{ km}^2$ ^a, well within the precision requirement. Although the instruments are at different spatial resolution, we do not find an large differences in cloud contamination (Section S2.3.1), or biases caused by sub-pixel inhomogeneities in illumination (Section S2.3.2) and methane concentration (Section S2.3.3) between the two instruments.

^aCalculation based on central limit theorem. 0.15% translates to 2.85 ppb assuming a 1900 ppb XCH_4 . The precision of the sample mean reaches the requirement for ~ 150 pixels, which translates to $\sim 3 \times 3 \text{ km}^2$, assuming a $140 \times 400 \text{ m}^2$ native pixel size.

RC: *Certain sections of the paper could benefit from a more concise description, and the overall structure could be improved for clarity and better organization. Consider introducing additional subsections to achieve this.*

AR: We have implemented the majority of subtitle suggestions by the first reviewer, which should cover this point.

RC: *Consider to display the mathematical expression used to compute the squeeze factor in the forward model. Overall, provide some more details on the forward model (e.g. input quantities, etc.).*

AR: We have significantly expanded Section 1 of the supplement. It now contains a comprehensive description of the forward model.

RC: *Emphasize that the ISRF squeeze is a nominal fit parameter and clarify that the remaining bias is a result of defocusing, which cannot be resolved solely through the ISRF squeeze adjustment but necessitates an additional preprocessing step, such as PLS regression.*

AR: It already does say this in Section 4, explaining the need for the cross track regression.

It is unlikely that squeezing the tabulated laboratory ISRF fully accounts for the change in ISRF shape induced by defocusing. The gradual drift in instrument focus may lead to a time-dependent XCH_4 cross track bias, which we attempt to derive using a "small area approximation" (O'Dell et al., 2018).

RC: *The bias analysis would benefit from additional details regarding the underlying assumptions and background information.*

The additional changes recommended by reviewer 1 for clarification in the section hopefully address this comment.

3. Specific Comments

RC: *63: Consider to add some recent literature sources on airborne methane retrieval (e.g. methane by HySpex)*

AR: We have added HySpex to the list of airborne sensors already cited

Recently instruments designed to detect high concentrations of CH_4 in individual methane plumes have been deployed on aircraft (AVIRIS-Thorpe et al. (2012), AVIRIS-NG-Thorpe et al. (2016), HySpex-Hochstaffl et al. (2023)) and satellites (Sentinel 2-Varon et al. (2021), GHGSat-Jervis et al. (2021), CarbonMapper-Shivers et al. (2021), PRISMA-Guanter et al. (2021), EnMAP-Roger et al. (2024))

And MAMAP later:

The CO_2 -Proxy method was first used from an airborne platform by the MAMAP instrument (Krings et al., 2011; Gerilowski et al., 2011), ...

RC: *99: Could you provide some brief insights into the command chain involved in operations like near realtime satellite commanding, which relies on forecasts and other factors? I*

AR: I have added a citation to the PhD thesis that provides the details of the scheduling system (Benmergui, 2019).

RC: *132: The accuracy of the proxy method could potentially be compromised if there is gas flaring occurring in close proximity?*

We have updated the supplement (Section S2.2) to assess errors caused by CO_2 co-emission from gas flares. We estimate based on currently known distributions of gas flaring efficiencies that flare emissions from US oil and gas basins will be underestimated by 8-16% depending on the basin. We are currently assessing alternate approaches for situations where we expect local CO_2 enhancements including using the unnormalized columns, or proxy-normalization from the O_2 singlet-delta band.

RC: *137: The MethaneAIR ground pixel size significantly differs from the nominal resolution of MethaneSAT. Any conclusions for MethaneSAT need to address assumptions and limitations in such a projection.*

AR: This is now addressed in Section 2.3 of the supplement, as already discussed in the general comments.

RC: *185: Consider to be more explicit. But if I understand correctly, there are a total of 19 layers from the Bottom of the Atmosphere (BOA) to the Top of the Atmosphere (TOA), with 13 of these layers situated within the troposphere. 18 + Table 1: Why scale all 19 layers when the enhancement primarily originates at or near the surface and likely remains concentrated in the lower layers for several kilometers, especially under steady wind and stable atmospheric conditions?*

AR: The enhancement above background occurs in the lowest layers, however for an individual sounding there is also the bias in the a priori background. The observed CH₄ line absorption depths are larger for the same increase in CH₄ molecular density for lower layers due to the effect of pressure broadening. Thus if the background was under/overestimated by the prior, scaling only the surface layer will under/overestimate the column XCH₄. The reverse is true if we scaled the entire column.

We currently optimize the 19 levels, but they are constrained by a prior covariance matrix (figure S1) that specifies correlations between the levels. This is the approach used by other satellite proxy retrieval algorithms (e.g. SCIAMACHY - Frankenberg et al. (2006), GOSAT - Parker et al. (2020)). Here we have adjusted the prior covariance such that the response to boundary layer differences is close to 1:1 (Averaging kernels, Figure S2).

RC: *199: An Instrument Spectral Response Function (ISRF) squeeze factor of less than 1 typically indicates squeezing, while a factor greater than 1 signifies stretching. So, ISRF squeeze < 1 means squeezing, and ISRF squeeze > 1 means stretching? Be more explicit.*

AR: Added sentence after equation:

From Equation 3, x_{sqz} values below/above unity correspond to stretching/squeezing the tabulated ISRF respectively. ”

RC: *203: Where is this shown? Eq.(3): Consider to include the complete formula for the squeeze factor.*

AR: Figure 3 - middle panel - I have put it in brackets after the statement. Eq. 3 is the complete formula for the squeeze factor.

RC: *220: “... high optical depth,...”? Fig. 4: Is it plausible or reasonable to assume that XCH₄ (XCH₄ typically refers to column-averaged dry-air mole fraction of methane) is enhanced at the position of the cloud?*

AR: Yes it’s a typo for high optical depth - now fixed

The paragraph refers to “CH₄ vertical column densities (VCDs)” not XCH₄ i.e. the vertically integrated number density (molecules/unit area). High optical depth clouds will in most cases have a light path shortening effect, leading to a decrease in CH₄ VCD relative to the value computed from the a priori. This is in essence the principle used by the OCO₂ A-band cloud processor. The only difference is that there is a higher uncertainty in the CH₄ relative to the prior. We estimate the background uncertainty using the data pre-screened using data from the O₂ band (where it spatially overlaps), and set this as the baseline to account for a priori CH₄ VCD uncertainties. We estimate a probability of a cloud based on the distance the retrieved CH₄ VCD is away from this baseline. We do the same for CO₂ and combine the values from all 3 (O₂, CH₄, CO₂) using a naive Bayes classifier. The full method will be available in a forthcoming publication.

RC: 264: Is “mechanistically” the right term?

AR: See comment to Reviewer 1. Changed sentence to:

Since there is an underlying physical connection between the XCH₄ cross-track bias and ISRF squeeze parameters, ...

RC: 268: “... 10 s of observations”? Fig. 5: In (a1) and (a2), where is the representation of the XCH₄ bias located or depicted?

AR: It should be Fig. 5 (c2) - text updated

As the noise in retrieved ISRF squeeze parameters is lower than the retrieved XCH₄, this will also improve the precision of cross-track bias prediction compared to direct application of the values in Figure 5 (c2).

RC: 276: Repeating “valuable”

AR: Fixed

RC: Fig. 7: Check first sentence in caption. Add XCH₄ label to colorbar. Show Beta from Eq. (5) or at least add some information in the caption that helps to better relate the figure with Eq. (5).

AR: Added "XCH₄ Bias" label to colorbar.

I have updated the caption in Figure 7:

XCH₄ cross track bias estimate with the small area approximation (left) and subsequently refined using the PLS regression model (right). The PLS regression model (Equation 5) uses the retrieved ISRF squeeze factors to predict the data in the left panel, in order to preserve only sources of variability related to the temperature-induced defocusing effects.

RC: 318: Clarify.

AR: Smaller particles lead to larger angstrom exponents, suggesting that even though smoke could be seen at visible wavelengths, it did not scatter sufficiently in the SWIR where the observations were made.

RC: 341: Was the TROPOMI L2 product destriped as part of the processing, or was it delivered already destriped? My assumption is that they provide a destriped product.

AR: They do not (or at least did not at the time of submission). I speculate it is an operational processing scheduling issue. If a product requires n previous days of observations to make the correction, then this means that production of the final version of that file would be delayed by that amount of time.

RC: 369-372: The XCH₄ albedo dependence analysis in Fig. 12 is conducted only for a single scene. Is this sentence required?

AR: The scene is representative of data from the campaign. The low sensitivity to surface features is important to emphasize, as it is critical for enabling quantification of methane emissions below the plume detection limit. This is an overarching goal of the MethaneSAT/MethaneAIR project.

RC: 377: Where to find Fig. S3?

AR: In the supplement - I think this is standard notation for this, but open to suggestions.

RC: **401: Review the sentence (IME is not directly a plume detection method).**

AR: Changed to:

The filter was chosen for its favorable properties, such that the resulting smoothed XCH₄ fields could be used to estimate CH₄ point source emissions (Q) without inducing additional bias. Here and for MethaneSAT, the integrated mass enhancement (IME) method (Frankenberg et al., 2016; Varon et al., 2018) is the primary method used to estimate Q :

RC: **Fig. 8: Add more details to the caption. The stripes are in the along-track direction due to the cross-track bias? Do I see multiple parallel flight tracks here?**

AR: Added context to flight path:

Here the aircraft is traveling in a clockwise loop, with the northern segments overlapping to target a controlled release.

RC: **Fig 9 Fig. 10: Was the averaging kernel actually considered in the comparison? It may be beneficial to show the formula to accommodate the varying vertical.**

AR: The averaging kernel can be used to adjust both sensors to a single prior - however in this case they are both using almost identical GGG2020 profiles (the only difference is that they are calculated with GEOS-FP vs. GEOS-FPIT met products, the latter being a frozen GEOS-FP release to maintain consistency for long-term datasets). If there was a coincident in situ column measurement then both could be compared to that, but we do not have this.

The other alternative is to estimate the distribution of expected differences using an ensemble estimate to anchor both soundings to - see Rodgers and Connor (2003), section 4.3. In this case you still need to define the probability distribution of the ensemble. Another approach for accounting for the vertical sensitivity difference would be to smooth the retrieved EM27 profiles by the MethaneAIR averaging kernels. However this will not factor in errors in the EM27 averaging kernel, and since its stratospheric values are changing significantly between some of the overpasses we thought it easier to just discuss the associated smoothing errors in the context of GGG2020 uncertainties. If the reviewer believes this is worthwhile, we can update the figure with this additional method.

RC: **Fig 12: Consider providing a brief description of the y-axis label in the caption. Additionally, could you explain why the lines do not exhibit a consistent trend towards either higher or lower values? If scattering is the underlying process responsible for this bias, it's puzzling why it does not consistently manifest as either a positive bias (indicative of multiple scattering) or a negative bias (indicative of single scattering).**

AR: The description is in the caption - updated to explicitly call it that

XCH₄ bias (y-axis) is derived by subtracting the mean XCH₄ for albedos between 0.19–0.21.

The discussion of the trend is already in the discussion of the figure in Section 5.3 - the reason for the slight upward trend at lower albedos is regularization bias (L375 in discussion paper). The bias for high albedos is due to a few unfiltered clouds. This is why there is not a consistent sign, as it is not one phenomenon.

Our main point was that the albedo-induced bias is less for the proxy-approach compared to other XCH₄ retrievals (either low res spectrometers like AVIRIS whereby the spectral information is difficult to separate from albedo) or strong CH₄ band full-physics retrievals like TROPOMI, that require aerosol optical property assumptions to connect the CH₄ estimate to the spectrally separated light-path constraint.

RC: 390: *Please provide details on how the value of 35 ppb was determined. Is it based on the standard deviation or another statistical measure? Fig 14: Check axis labels on right panel.*

AR: It is the precision determined by the standard deviation of the measurements in Fig 12. The manuscript has been updated to make this explicit

We estimate the precision of the 5×1 aggregated retrievals of 35 ppb, by taking the the standard deviation of the XCH₄ retrieved over background locations used in Figure 12.

The Axis label on the right panel is now fixed.

RC: 545: *The resolution is similar to TROPOMI's resolution (at least it is in the same order of magnitude.)*

AR: The 0.15% precision refers to the target precision at a scale of 3x3 km². The native MethaneSAT pixel is 400x130m² (change subject to final orbit altitude). In contrast, TROPOMI's precision for a single 5.5×7 km² pixel is 0.8%. The point of the sentence was to say what the threshold spatial scale is for detecting small XCH₄ gradients (above 3 ppb).

RC: 545: *Provide more context or specify where the analysis yielding the result of 0.15% is located? Additionally, it would be helpful to understand the assumptions made to arrive at this conclusion.*

AR: We have updated the paragraph to provide the context for the 0.15% target threshold, which was based on emission inversion observing system simulation experiments. The way the instrument precision was reached was based on precision estimates from a linear sensitivity analysis (Section S2.1). The estimate that the precision will be achieved at the 3×3 km² spatial scale just follows from the central limit theorem, as discussed earlier in these responses.

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