

## How can we trust TROPOMI based Methane Emissions Estimation: Calculating Emissions over Unidentified Source Regions

The author presents a methodology for estimating methane emissions using TROPOMI data while accounting for observational uncertainty. These uncertainties are crucial, as they can significantly influence emission estimates. However, there are several critical aspects of the methodology that need to be carefully reviewed.

1. Selecting pixels with  $QA > 0.5$  may introduce artefacts, potentially increasing uncertainty in the emission estimates. Rather than relying solely on this threshold, did you explore the use of AOD and albedo filters as recommended by Schuit et al. (2023) and Nesser et al. (2024)? If so, how did these alternative filtering approaches impact your results? I strongly recommend using only pixels with  $QA = 1.0$ , as lower QA values may include retrieval artefacts. Additionally, did you consider using the blended TROPOMI+GOSAT product, which reduces biases through the integration of GOSAT data? This could further enhance the robustness of your emission estimates.
2. Figure 2: Typically, pixels classified as water surfaces—especially those near coastal areas—are excluded due to their high uncertainty and potential for retrieval errors. Including TROPOMI pixels over water bodies can lead to unreliable or biased emission estimates, as these pixels often suffer from issues related to surface reflectivity and retrieval sensitivity. Additionally, the manuscript does not show a 2D map of TROPOMI  $XCH_4$  in the Waliguan region and Permian Basin, which would help in evaluating the spatial context and data quality. It would also be beneficial to include maps of supporting variables such as albedo, AOD and surface pressure in this region to assess the robustness of the retrieval and filtering process. I recommend adding these visualizations and clarifying how water-body pixels were handled in your analysis. Can you also add the TROPOMI observational density maps?
3. Lines 203–205: TROPOMI measures the total column-averaged dry-air mole fraction of methane ( $XCH_4$ ), whereas the Waliguan station provides surface-level  $CH_4$  concentrations. These are fundamentally different metrics, so differences between them should not be interpreted directly as errors. For a valid comparison, TROPOMI  $XCH_4$  should be compared with total column measurements from ground-based instruments like TCCON. Please clarify whether the comparison shown is based on grid-to-grid analysis or a 50 km spatial average of TROPOMI data; this should be stated clearly in the main text or Figure 1 caption. Additionally, both datasets show a rising methane trend, which is encouraging and should be highlighted in the results.

Regarding the 10% random perturbation applied, it is inappropriate to base this on differences between surface  $CH_4$  and TROPOMI  $XCH_4$  due to their different measurement scopes. Instead, perturbations simulating satellite uncertainty should rely on differences between TROPOMI and independent total column observations such as TCCON, to maintain physical consistency and justification.

4. While the manuscript addresses uncertainties related to TROPOMI observations, it does not account for uncertainties in wind speed, which are a critical component in top-down emission estimation. How does the use of boundary-layer averaged wind speed influence the emission estimates in your methodology? In the remote sensing community, it is standard practice to use multiple wind products and assess their associated uncertainties. However, I could not find any discussion or quantification of wind-related uncertainty in the current manuscript. Including this analysis would significantly strengthen the credibility and completeness of the results.
5. It is unclear why the robustness of the filtering method diminishes when the assumed TROPOMI uncertainty is increased to 20%. Could you clarify how these uncertainty threshold values were selected? Lines 260–264 are particularly difficult to follow and

should be revised for clarity. You mention that the  $R^2$  value decreases under the 20% uncertainty assumption—please explain the underlying reason for this reduction. It would be helpful to elaborate on the relationship between the assumed uncertainty level and the resulting  $R^2$  value.

6. In Figure 4, the bias after panel (e) is lower (0.56) compared to the filtered case (-1.62) when a  $\pm 10\%$  perturbation is applied to TROPOMI XCH<sub>4</sub>. However, the  $R^2$  value remains largely unchanged between these cases. These metrics alone do not sufficiently demonstrate how the filtering or threshold choices influence the emission estimates. It would be helpful to provide additional analysis or metrics that better illustrate the impact of these filtering options on the accuracy and reliability of the emission estimations.
7. Section 2.4 is difficult to follow. Please consider splitting it into spatial filtering (removing grid cells with emission rates below 21.2  $\mu\text{g/m}^2/\text{s}$ ) and temporal filtering. Also, clarify how the thresholds of 17, 25, and 31  $\mu\text{g/m}^2/\text{s}$  were chosen—are these related to specific percentiles? If Figure 3 illustrates the method, please reference it or include a schematic for clarity.
8. Have you considered using the median instead of the mean for the spatial filtering, since the mean can be influenced by regional transport and outliers? How does the emission estimate change when using the median?
9. Figure 6 d,e, f is missing.
10. Please provide the specific methane emission estimates reported by Cusworth (2021). How do your estimates compare to bottom-up inventories over the Permian Basin? Additionally, how do your results differ from other inversion-based CH<sub>4</sub> emission estimates in this region? There are also high-resolution satellite products like GHGSat and Carbon Mapper for facilities in the Permian Basin—how does your comparison with these datasets look? Do your estimates fall within their uncertainty ranges, or are there significant discrepancies?
11. The manuscript should include a clear quantification of the overall uncertainty associated with your method. Please provide an explicit uncertainty estimate and discuss its implications for your results.
12. Line 265 to 270: You mention that the largest positive values have been filtered out. Have you examined whether these locations correspond to known biases in surface albedo or aerosol optical depth (AOD)? High albedo or AOD can cause significant retrieval errors that might explain some of these extreme emission values. I strongly recommend incorporating supporting variables such as AOD, surface pressure, and albedo in your analysis. Without these contextual data, it is difficult to distinguish genuine emission signals from noise. Including these layers would enhance the transparency and robustness of your filtering method and better justify your data processing decisions.

#### Specific comments:

1. In Introduction, provide a detailed description of the inversion model used in this study and specify the geographical area where the inversion was applied. Instead of broadly stating that many studies use simple or complex models to estimate TROPOMI-based emissions, include specific examples of inversion models along with the regions they have been applied to, to better contextualize your approach.
2. Methodology: What type of trained model is used to calculate emissions? Are you referring to a machine learning approach or another type of model?
3. Line 127: You mention “such as the transport term and diffusion term in our equations and the divergence method used by others.” Please specify who these “others” are by citing relevant studies or authors.
4. Line 131: The example given about XCH<sub>4</sub> values and uncertainties is confusing. With values of 1800 and 1900 ppb and 10% uncertainty, the ranges should be 1620–1980 ppb and 1710–2090 ppb respectively. Given this, how could the gradient become

negative or zero? Subtracting the lower and upper bounds still results in a positive gradient ranging from 90 to 110 ppb. Please clarify this point.

5. Line 154: What traditional technique are you referring to here? Please be specific.
6. Line 155: Is the perturbation applied consistently across all grid points or randomly across the chosen study domain?
7. Line 167: You state, “any positive value of the same magnitude or smaller is also due to uncertainty.” Does this refer to the 21.2  $\mu\text{g}/\text{m}^2/\text{s}$  threshold or another value? Please clarify.
8. Line 177: What do you mean by “overlap between  $\text{CH}_4$  and other species which are not resolved”? Which species are you referring to? Please specify.
9. Figure 4: The x-axis and y-axis labels are difficult to read—please increase their font size for better visibility. Additionally, the figure caption is confusing and does not clearly indicate which descriptions correspond to each subplot. I recommend revising the caption to be clearer and more concise, explicitly linking each part of the description to the respective subplots.
10. Line 259: Please separate the slope,  $R^2$  value, and bias for clarity. Also, provide context explaining what Figures 4c and 4d specifically illustrate to help readers better understand their significance.
11. Line 272: The statement about removing negative emission values or using the absolute value of the gradient is incorrect and needs revision. Studies like Maasakkers et al. (2021) and Shen et al. (2021) use inversion methods that do not apply the absolute value to the gradient. In fact, negative emissions commonly appear in normal inversion results but are retained in the analysis rather than removed.
12. Line 273: The phrase “same analysis approach” is vague. Please specify the exact method or approach you are referring to for clarity.
13. Line 37: Should it be “surface warming” or “global warming”? Please clarify.
14. Line 39: Use “gases” instead of “gasses.”
15. Line 43: Provide the full names of TROPOMI, GOSAT, and SCIAMACHY before using the acronyms.
16. Line 44: Spell out the full forms of AGAGE, WMO, and TCCON.
17. Line 50: Use “extensive work to estimate uncertainty” instead of “extensive work on uncertainty.”
18. Line 58: Specify what kind of in-situ processing and other processes are referred to; please explain in detail.
19. Line 62: Clarify what “significant non-linearity” means and provide quantitative uncertainty values for emission estimates.
20. Line 69: Define “clean area.” Do you mean a background area without emissions?
21. Line 72: Specify the type of threshold and filter used, or refer to the section where this is detailed.
22. Lines 87–88: Clarify the phrase “The XCH4 retrieval used herein (version 2.4.0 Level 2) relies on a physical algorithm that factors in surface and atmospheric scattering.” What exactly does this mean?