Review of “Extension of the S5P-TROPOMI CCD tropospheric ozone retrieval to mid-latitudes,” by Maratt Satheesan et al. 2025

Maratt Satheesan et al. present a new satellite algorithm to retrieve tropospheric column ozone (TCO) defined as surface–450 hPa from S5P/TROPOMI across 60° S–60° N. The method selects a local cloud reference sector (radius adaptively grown from ~60 to 600 km) to estimate above-cloud column ozone (ACCO) locally, adjusts ACCO to a common upper layer (450 hPa), and then derives grid-box TCO for nearby clear pixels by subtracting this ACCO from the total column. The algorithm operates in two modes: CLCD-C (climatology-based) and CLCD-T (Theil–Sen regression using cloud-top variability). Monthly TCO fields for 2018–2022 on a 0.5°×0.5° grid are validated against 36 ozonesonde sites, with an overall mean bias of about 0.6 DU and dispersion of about 2.5 DU reported. The resulting TCO product could be useful for trace-gas studies.

Major comments

1. The manuscript is dense. Please consider shortening background and moving secondary figures to SI to focus the main text on algorithm, validation, and key findings.

2. Product definition and comparability
   Please consolidate the product definition in a single table: vertical layer (surface–450 hPa), grid (0.5°×0.5°), temporal averaging (daily box means → monthly composites), and coverage. Include a side-by-side comparison with existing TCO products—e.g., TROPOMI O3_TCL (surface–270 hPa), OMI/MLS (surface–tropopause), and one reanalysis—highlighting differences in layer definitions, resolution, and known biases. Provide diagnostic maps of (surface–450 hPa) − (surface–tropopause) and (surface–450 hPa) − (surface–270 hPa) so users can reconcile your product with traditional TCO definitions.

3. Algorithm transparency & reproducibility
   (a) Document the local cloud sector growth (start radius, increment, stop criteria, near-overcast thresholds) and whether pixels are area- or quality-weighted. Provide a sensitivity study for sector radius caps (60/300/600 km) on ACCO stability.
   (b) Please justify representativeness when sectors exceed several degrees in longitude/latitude (e.g., at 60° N, 600 km is about 10° of longitude). Terrain-stratified validation (plains vs mountains) would help quantify impacts over complex topography.
   (c) Specify all homogeneity criteria for total ozone and report rejection rates. Clarify time mapping: is ACCO derived and applied to clear pixels within the same orbit/day, or via compositing? Also state the ozonesonde measurement time and the collocation time window relative to the S5P overpass.
   (d) Provide per-region CLCD-C vs CLCD-T usage fractions through the year.

4. Cloud distance & 3D cloud radiative effects
   Define distance-to-cloud-edge formally (measurement space, units, how edges are detected). In Fig. 6f the mean distance spans from 50 to more than 400 km; please explain this range and any sharp transitions. Quantify the CLCD-TCO residuals vs edge distance diagnostics to reveal 3D effects. Clarify handling of cirrus and multi-layer clouds and their impact on effective cloud pressure.

5. Uncertainty
   Report **relative** as well as absolute uncertainty, and decompose errors into random and systematic terms. Provide the frequency of negative ACCO/TCO, and guidance on QC thresholds to achieve typical targets (e.g., ≤10% relative error for monthly 0.5° boxes). Please discuss error correlation within sectors (shared ACCO) and implications for averaging.

6. Validation & additional comparisons
   Clarify collocation windows (space/time) and whether validation uses daily or monthly aggregates (or both). Consider replacing crowded multi-panel plots with site-wise summary bars (bias, SD, r, slope) grouped by latitude/season/cloud regime, and add a map of sites colored by bias. Include layer-matched comparisons with TROPOMI O3_TCL (tropics), OMI/MLS climatology, and a reanalysis (GEOS-CF/CAMS).

7. Bias analysis & future improvements
   The manuscript explains biases largely on a case-by-case basis, which makes it difficult to identify clear priorities for improvement. Please outline a concrete plan for future algorithm development—specifying the main bias sources to be addressed, the diagnostics to be added, and the methodological changes you anticipate implementing.

Specific comments

P.1 l-22: Please report relative as well as absolute TCO uncertainty (e.g., % of the column) and state recommended QC thresholds for “usable” data at low-TCO sites.

P4 l-92: Specify the spatial/temporal resolution and version of the cloud parameters, and whether they are resampled to the ozone grid. Clarify consistency between cloud and total-ozone inputs.

P4 I-100: Provide monthly variance (and sample size) of ozonesonde TCO at each station. Clarify whether sonde sampling variance is included in the retrieval uncertainty (the current Eq. (1) does not indicate this).

P5 l-131: State the years used for climatology and discuss representativeness (e.g., trends/decadal changes). Include a sensitivity to the climatology epoch.

P5 l-132: Ten degrees is coarse for 0.5° boxes. Consider a finer-resolution or more recent climatology and quantify the impact on TCO.

P5 l-140: Justify the cloud-fraction and cloud-top-height thresholds and provide a short sensitivity analysis.

P6 l-150: Clarify handling of cirrus, multi-layer**,** low clouds (e.g., low optical thickness, clouds below 2 km). State any screening and its effect on coverage.

P6 l-164: Please clarify the dataflow: Are retrievals performed daily per 0.5° box and then aggregated to monthly, or are any steps done on monthly composites?

P6 l-165: Report how often and under what conditions negative ACCO/TCO occur.

P8 Figure 3: Please clarify the total number of TROPOMI footprints contributing to each 0.5°×0.5° grid box.

P11 Figure 6: (e) Does the cloud reference sector change seasonally for a given box? If this is the case, please provide the distribution of selected radii by month and region. (f) Define **-** distance-to-cloud edge precisely (units, edge detection). Explain the sharp transitions and how mean distances can vary from ~400 km to ~50 km. Quantify how often boxes have no clouds within ≥4° and how such scenes are handled.

P12 l-212: Provide monthly ozonesonde TCO variance and collocation counts used in each comparison.

P13 l-241: Please standardize product naming (e.g., CLCD-TCO) across the text, tables, and figures. For example, Table 1 uses CLCD-TCO, whereas Figure 8 uses TROPOMI–sonde. Use consistent terminology and explicitly indicate the vertical layer (e.g., surface–450 hPa) in figure labels/captions so it's clear whether the comparison refers to total column ozone or the TCO up to 450 hPa.

P13 l-269: Please specify the kind of possible issues.

P15 Figure 7 and P21 Figure 9: Increase symbol sizes and axis fonts; choose more distinct line colors/symbols.

P16 Figure 8: The small multiples are hard to parse.

P17 l-281: Where high positive TCO bias is linked to remote low-level clouds, test whether the source is (i) ACCO estimation mode (CLCD-C vs CLCD-T) or (ii) the ACCO to ACCO above 450 hPa conversion. Show targeted sensitivity tests.

P18 l-315: Describe the atmospheric profiles and weighting-function used to convert ACCO to ACCO above 450 hPa, and quantify this term's contribution to the uncertainty budget beyond climatology.

P20 l-390: State that whether ozonesonde profiles are convolved with the same weighting (or simple box integration, as appropriate) before comparing with the derived TCO.

P 28 Figure 14: Explain why the latitude range is 30° S–30° N here while other figures (figures 5 and 6) use 60° S–60° N, or harmonize the ranges.

P29 Figure 15 and P30 Figure 16, 17: The maps show pronounced topographic signatures (e.g., Tibetan Plateau, Rocky Mountain) with TCO values apparently lower than those reported by Liu et al. (2022) and Xu et al. (2024). Some differences may stem from layer definitions (surface–450 hPa here vs surface–tropopause or other in those studies). Please consider: (i) provide layer-matched comparisons by converting your product to surface–tropopause and surface–270 hPa where feasible, or by integrating the reference products to surface–450 hPa; (ii) include cross-comparisons with reanalyses (e.g., GEOS-CF, CAMS) at the same layer/grid. These additions would better demonstrate the robustness of the retrieval over complex topography.

References

1. Liu, J., Strode, S. A., Liang, Q., Oman, L. D., Colarco, P. R., Fleming, E. L., et al. (2022). Change in tropospheric ozone in the recent decades and its contribution to global total ozone. Journal of Geophysical Research: Atmospheres, 127, e2022JD037170. https://doi.org/10.1029/2022JD037170
2. Jian Xu, Zhuo Zhang, Lanlan Rao, Yapeng Wang, Husi Letu, Chong Shi, Gegen Tana, Wenyu Wang, Songyan Zhu, Shuanghui Liu, et al. Remote Sensing of Tropospheric Ozone from Space: Progress and Challenges. J Remote Sens. 2024;4:0178. DOI:10.34133/remotesensing.0178