Supplement Materials for

Air pollution satellite-based CO₂ emission inversion: system evaluation, sensitivity analysis, and future perspective

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Text S1. Tests affecting NO\textsubscript{x} and CO\textsubscript{2} emissions result in similar impacts

Among tests, Res\_2×2.5 and 2021\_base are the most influential ones, triggering $RC_\text{σ} \pm 1\sigma$, of -2.8%±6.2% (-1.2%±6.0%) and 0.5%±8.6% (-0.6%±6.9%) in daily national total NO\textsubscript{x} (CO\textsubscript{2}) emissions, respectively. Trop\_fill and Trop\_v2.3 come next, causing variations of 1.1%±5.3% (1.3%±3.9%) and -0.5%±6.7% (-0.4%±5.9%) in daily national total NO\textsubscript{x} (CO\textsubscript{2}) emissions. In contrast, $β_\text{[-20%, 20%]}$ leads to notable but consistent variations in NO\textsubscript{x} and CO\textsubscript{2}, linearly strengthening its impact as the adjustment amplitude increases, wherein $β_\text{-20%}$ triggers 3.0%±3.2% in NO\textsubscript{x} emissions and 2.6%±3.0% in CO\textsubscript{2} emissions (Fig. S5).

Text S2. Response of sectoral NO\textsubscript{x} emissions to tests

The residential sector is the most vulnerable to 2021\_base, with variations up to -6.0%±6.7% in daily NO\textsubscript{x} emissions. Residential emissions exclusively present sensitivity to 4\_sectors, thre\_04, and thre\_06, with variations of -6.1%±2.5%, 7.4%±7.8%, and -6.4%±5.6% in its NO\textsubscript{x} emissions, respectively. The industry and transport emissions are more sensitive to the $β_\text{[-20%, 20%]}$, with $RC_\text{σ} \pm 1\sigma$, up to 4.1%±4.5% and 4.5%±6.1% in NO\textsubscript{x} emissions under $β_\text{-20%}$. Res\_2×2.5 incurs the $RC_\text{σ} \pm 1\sigma$, of -8.3%±12.4% and -2.7%±8.8% in daily national NO\textsubscript{x} emissions in transport and power sectors, respectively.
Figure S1. The methodology of inversion system and the tests we introduced.
Sensitivity tests include prior (red labeled), model resolution (orange labeled), satellite data (blue labeled), and inversion system parameters (purple labeled). Detailed settings are seen in Tables 1 and 2.
Figure S2. The comparison of XGBoost filled TROPOMI and original TROPOMI NO$_2$ TVCDs in 2022. (a) shows the annual mean NO$_2$ TVCDs of original TROPOMI sampling. (b) shows the annual mean NO$_2$ TVCDs of filled TROPOMI using XGBoost method. (c) compares the daily national mean NO$_2$ TVCDs between original and filled TROPOMI. (d) shows the correlation between original and filled TROPOMI NO$_2$ TVCDs grid-by-grid.
Figure S3. **RC distribution of daily national total emissions under all tests.** The overall distribution of RC of daily national total emissions of NO\textsubscript{x} and CO\textsubscript{2} across all tests adheres to a normal distribution. For NO\textsubscript{x}, the mean (μ) and standard deviation (σ) are -0.03% and 2.92%, respectively, while for CO\textsubscript{2}, they are 1.90% and 4.08%. Given our discussion focusing on CO\textsubscript{2} emissions, 1σ = 4.0% is thus chosen as the threshold for distinguishing between consistent and inconsistent impacts.
Figure S4. An overview of consistency of tests’ impacts on (a) NO\textsubscript{x} and (b) CO\textsubscript{2} emissions across finer scales. The orange color signifies one standard deviation (1\textsigma), reflecting the degree of consistency in the impact of the corresponding test. A larger 1\textsigma indicates greater inconsistency. Sectoral emissions consistency is depicted on a daily scale, and spatial results are depicted on an annual provincial scale. The numbers within each grid represent the corresponding 1\textsigma on a certain dimension under tests.
Figure S5. Sensitivity of annual national total NO\textsubscript{x} and CO\textsubscript{2} emissions to $\beta$ and NO\textsubscript{x} emission factor. (a) and (c) present the estimated NO\textsubscript{x} emissions under ten-level gradient for $\beta$ and emission factor variations. (b) and (d) are plotted for CO\textsubscript{2} emissions as (a) and (c).
Figure S6. Ten-day moving average NOx and CO2 emissions in 2022 under different sensitivity tests. (a) and (b) present the ten-day moving NOx emissions under all tests and Base. (c) and (d) are plotted for CO2 emissions as (a) and (b).
Figure S7. Comparison of total (a) NO\textsubscript{x} and (b) CO\textsubscript{2} emissions in 2022 under various sensitivity tests. Label above each column refer to the corresponding tests.
Figure S8. Comparison of $\beta$ between Res_2$\times$2.5 and Base, 2021_base and Base. (a) and (c) compare the daily $\beta$ dynamics between Res_2$\times$2.5 and Base, and between 2021_base and Base, respectively. (b) and (d) present the spatial distribution of $\beta$ variance between Res_2$\times$2.5 and Base, and between 2021_base and Base, respectively. The gray shaded area is not calculated in this study.
Figure S9. Sectoral CO₂-to-NOₓ emission ratios in 2022 under Base inversion. Sectors are color coded.
Figure S10. Sectoral contribution to total NO\textsubscript{x} and CO\textsubscript{2} emissions in 2022 under Base inversion. Sectors are color coded.
Figure S11. The comparison of proportion attributing total TROPOMI-constrained NO\textsubscript{x} emissions to the residential sector. Black, red, and blue lines refer to the Base, thre\_40\% and thre\_60\% inversions, respectively.
Figure S12. The comparison of sectoral proportion of TROPOMI-constrained NO\textsubscript{x} emissions. Sectors are color coded. Deep color refers to the Base inversion, and light color represents the Res\_2×2.5.
Figure S13. Correlation between $RC_p$ in provincial annual total NO$_x$ and CO$_2$ emissions. Scatters in red, orange, blue, and purple colors show the results from the tests on prior, model resolution, satellite retrievals, and inversion system parameters, respectively.
Figure S14. Response of regional total NO\textsubscript{x} and CO\textsubscript{2} emissions under tests on a daily scale. (a), (b), (c), and (d) show the $\bar{R}_C \pm 1\sigma_r$ of daily NO\textsubscript{x} (deep color) and CO\textsubscript{2} (light color) emissions triggered by different tests in Jing-Jin-Ji clusters (Beijing, Tianjin, and Hebei), Inner Mongolia, Yangtze River Delta clusters (Shanghai, Zhejiang, and Jiangsu), and Guangdong.
Figure S15. Comparison of daily NO\textsubscript{x} and CO\textsubscript{2} emissions between Base and situation with iteratively optimized modification on NO\textsubscript{x} emission factors. (a) and (c) present the total and sectoral NO\textsubscript{x} emissions under Base (deep color) and situation with iteratively optimized modification on NO\textsubscript{x} emission factors (light color). (b) and (d) are plotted for CO\textsubscript{2} as (a) and (c).