Supplement Materials for

Air pollution satellite-based CO_2 emission inversion: system evaluation, sensitivity analysis, and future perspective

Hui Li[1,2], Jiaxin Qiu[1,2], Bo Zheng[1,2,*]

[1]Shenzhen Key Laboratory of Ecological Remediation and Carbon Sequestration, Institute of Environment and Ecology, Tsinghua Shenzhen International Graduate School, Tsinghua University, Shenzhen 518055, China.

[2]State Environmental Protection Key Laboratory of Sources and Control of Air Pollution Complex, Beijing 100084, China.

Correspondence to: Bo Zheng (bozheng@sz.tsinghua.edu.cn)

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- Texts S1 to S2
- Figures S1 to S15

Text S1. Tests affecting NO_x and CO_2 emissions result in similar impacts

Among tests, Res_2×2.5 and 2021_base are the most influential ones, triggering $\overline{RC_t} \pm 1\sigma_t$ of -2.8%±6.2% (-1.2%±6.0%) and 0.5%±8.6% (-0.6%±6.9%) in daily national total NO_x (CO_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_x (CO_2) emissions. In contrast, β_[-20%, 20%] leads to notable but consistent variations in NO_x and CO_2, linearly strengthening its impact as the adjustment amplitude increases, wherein β_20% triggers 3.0%±3.2% in NO_x emissions and 2.6%±3.0% in CO_2 emissions (Fig. S5).

Text S2. Response of sectoral NO_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_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_x emissions, respectively. The industry and transport emissions are more sensitive to the β_[-20%, 20%], with $\overline{RC_s} \pm 1\sigma_s$ up to 4.1%±4.5% and 4.5%±6.1% in NO_x emissions under β_-20%. Res_2×2.5 incurs the $\overline{RC_s} \pm 1\sigma_s$ of -8.3%±12.4% and -2.7%±8.8% in daily national NO_x emissions in transport and power sectors, respectively.

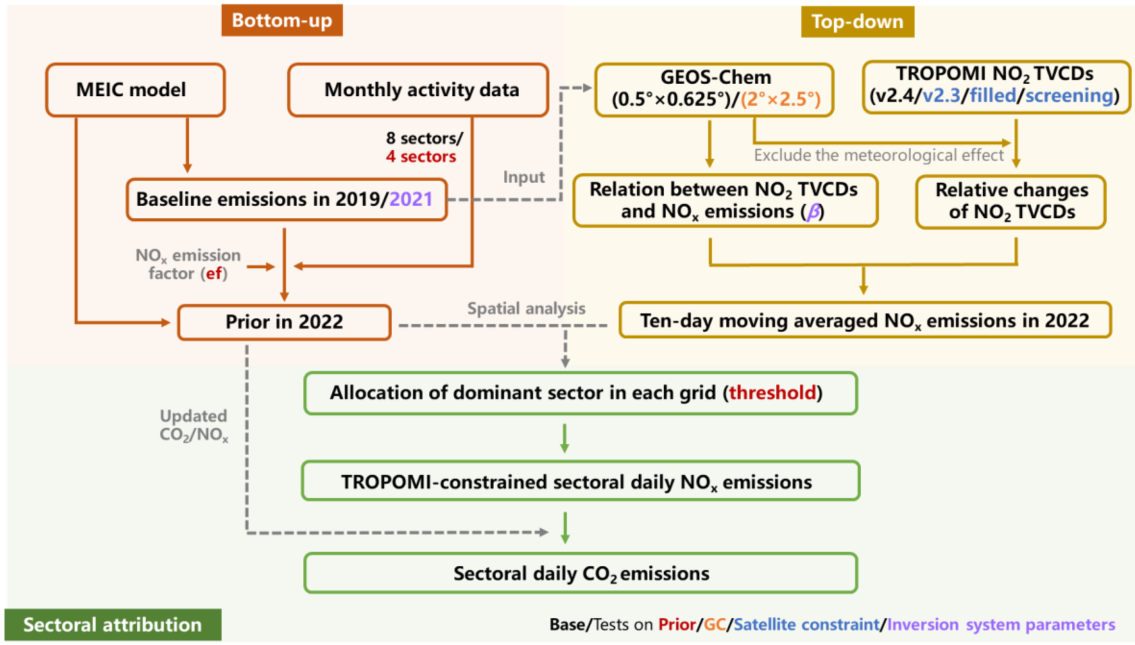

Figure S1. **The methodology of inversion system and the tests we introduced.** Sensitivity tests include prior (red labeled), model resolution (orange labeled), satellite data (blue labeled), and inversion system parameters (purple labeled). Detailed settings are seen in Tables 1 and 2.

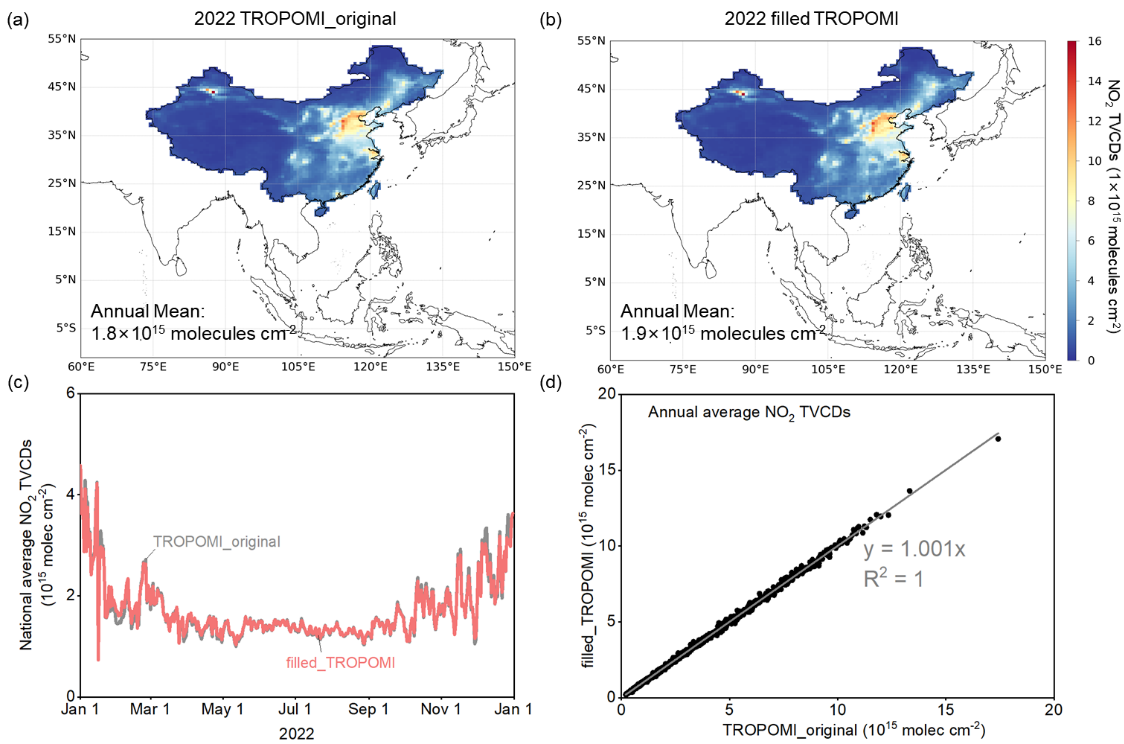

Figure S2. **The comparison of XGBoost filled TROPOMI and original TROPOMI NO_2 TVCDs in 2022.** (**a**) shows the annual mean NO_2 TVCDs of original TROPOMI sampling. (**b**) shows the annual mean NO_2 TVCDs of filled TROPOMI using XGBoost method. (**c**) compares the daily national mean NO_2 TVCDs between original and filled TROPOMI. (**d**) shows the correlation between original and filled TROPOMI NO_2 TVCDs grid-by-grid.

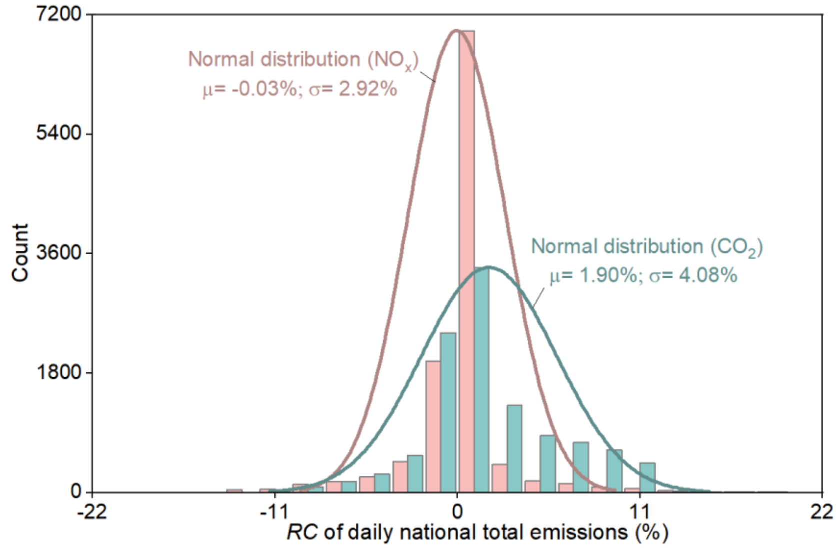

Figure S3. ***RC* distribution of daily national total emissions under all tests.** The overall distribution of *RC* of daily national total emissions of NO_x and CO_2 across all tests adheres to a normal distribution. For NO_x, the mean (μ) and standard deviation (σ) are -0.03% and 2.92%, respectively, while for CO_2, they are 1.90% and 4.08%. Given our discussion focusing on CO_2 emissions, $1\sigma = 4.0\%$ is thus chosen as the threshold for distinguishing between consistent and inconsistent impacts.

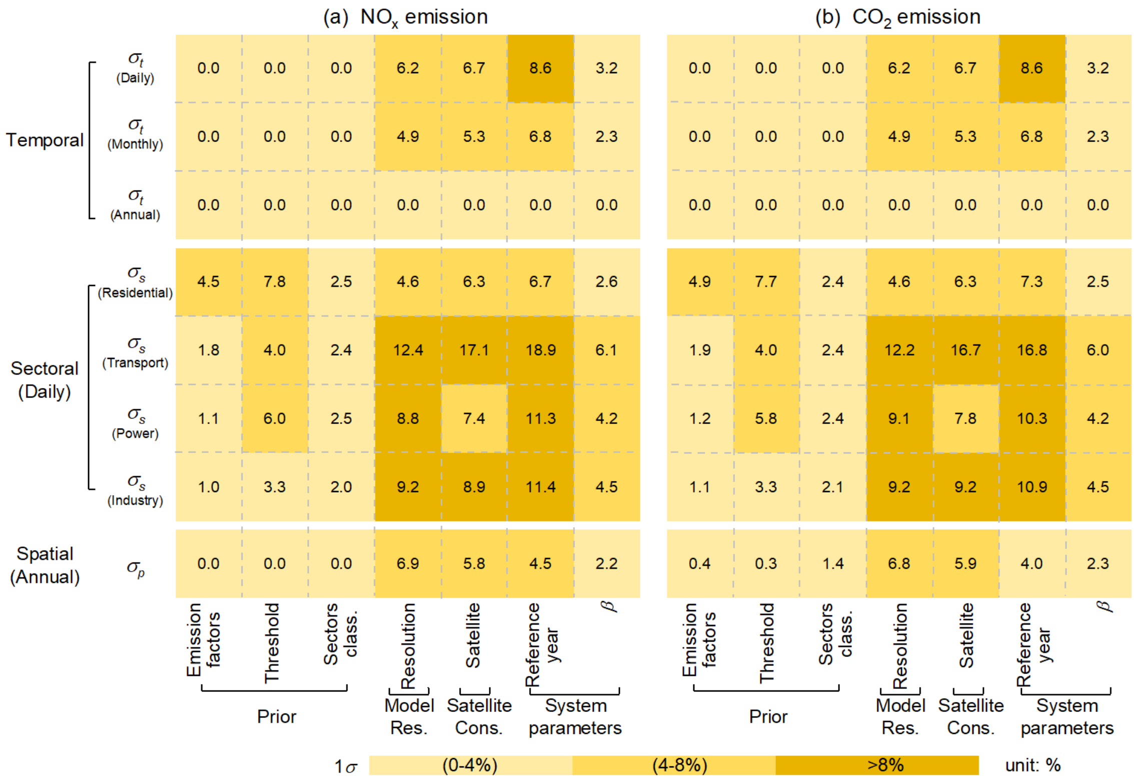

Figure S4. An overview of consistency of tests' impacts on (a) NO_x and (b) CO_2 emissions across finer scales. The orange color signifies one standard deviation (1σ), reflecting the degree of consistency in the impact of the corresponding test. A larger 1σ indicates greater inconsistency. Sectoral emissions 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 1σ on a certain dimension under tests.

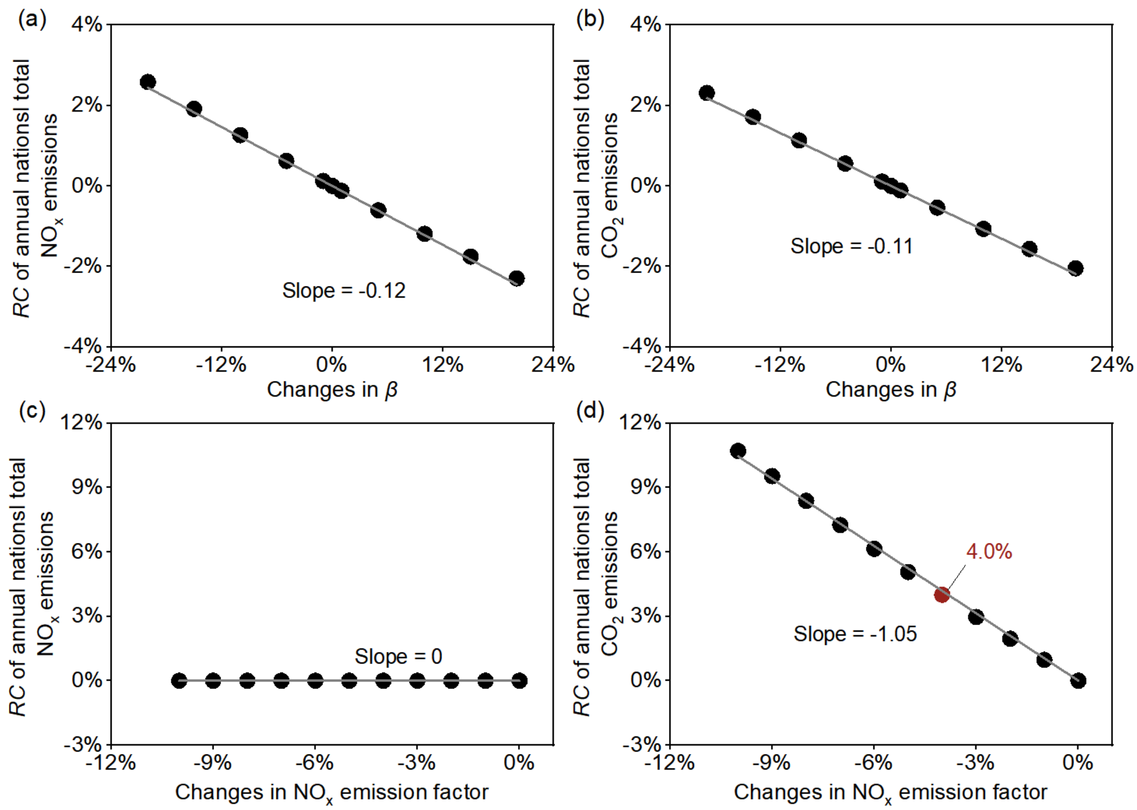

Figure S5. Sensitivity of annual national total NO_x and CO_2 emissions to *β* and NO_x emission factor. (**a**) and (**c**) present the estimated NO_x emissions under ten-level gradient for β and emission factor variations. (**b**) and (**d**) are plotted for CO_2 emissions as (**a**) and (**c**).

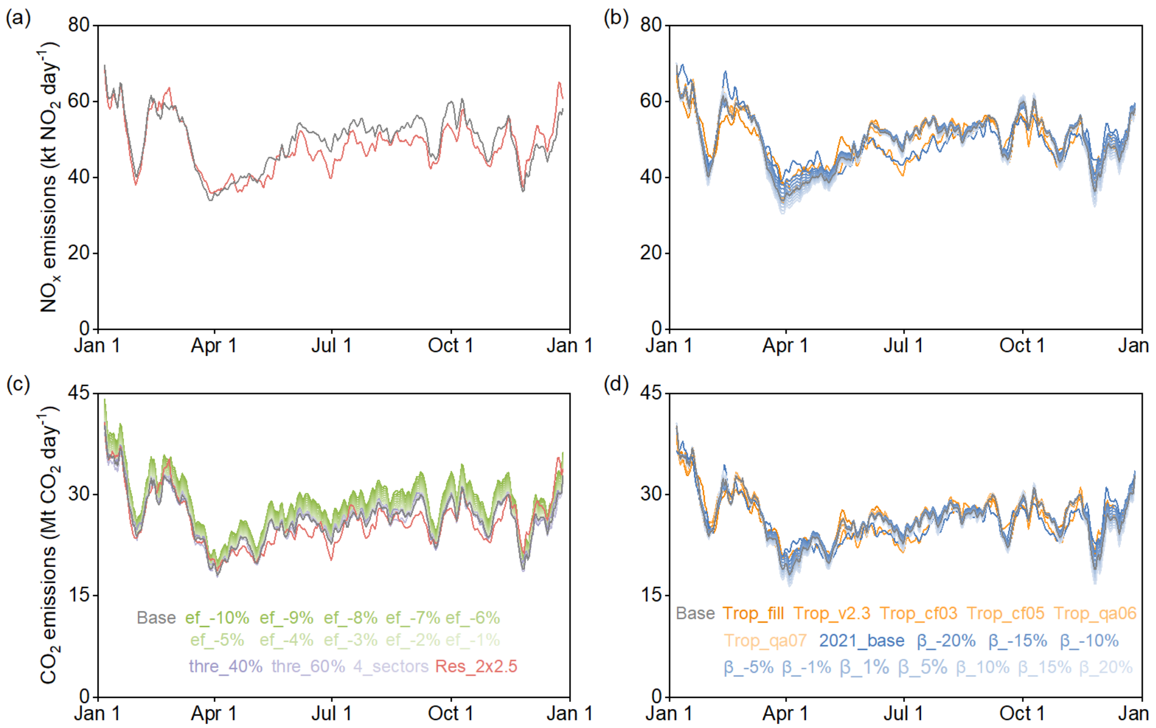

Figure S6. **Ten-day moving average NO_x and CO_2 emissions in 2022 under different sensitivity tests.** (**a**) and (**b**) present the ten-day moving NO_x emissions under all tests and Base. (**c**) and (**d**) are plotted for CO_2 emissions as (**a**) and (**b**).

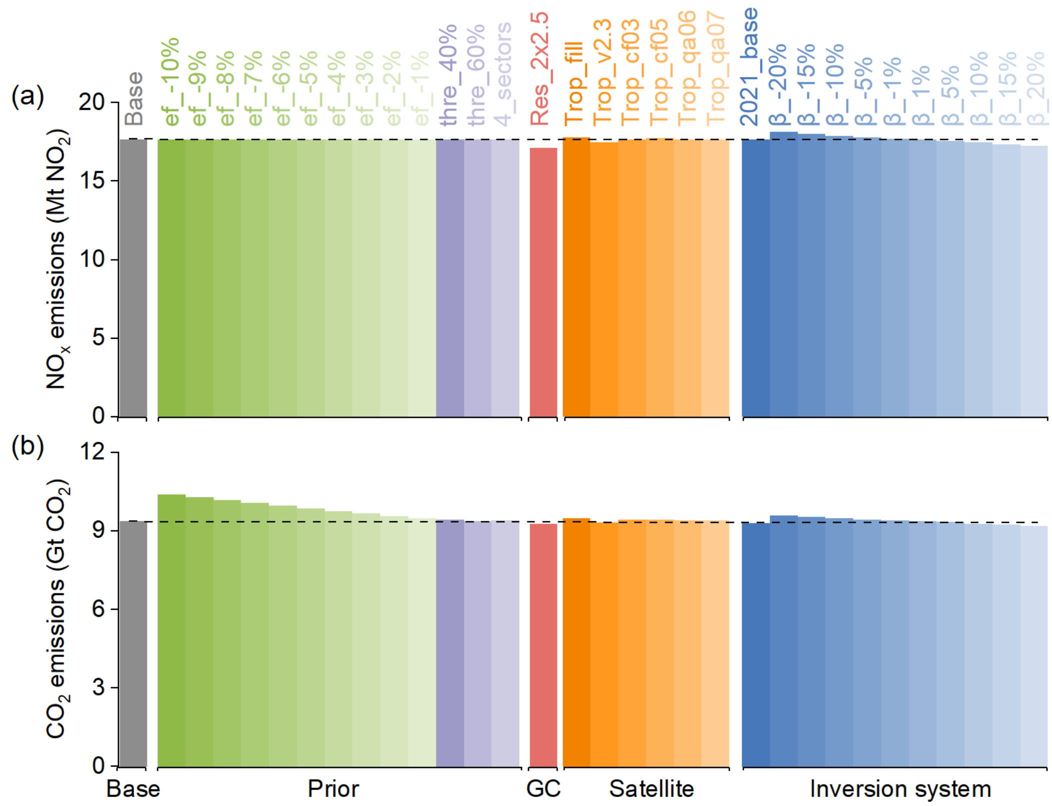

Figure S7. **Comparison of total (a) NO_x and (b) CO_2 emissions in 2022 under various sensitivity tests.** Label above each column refer to the corresponding tests.

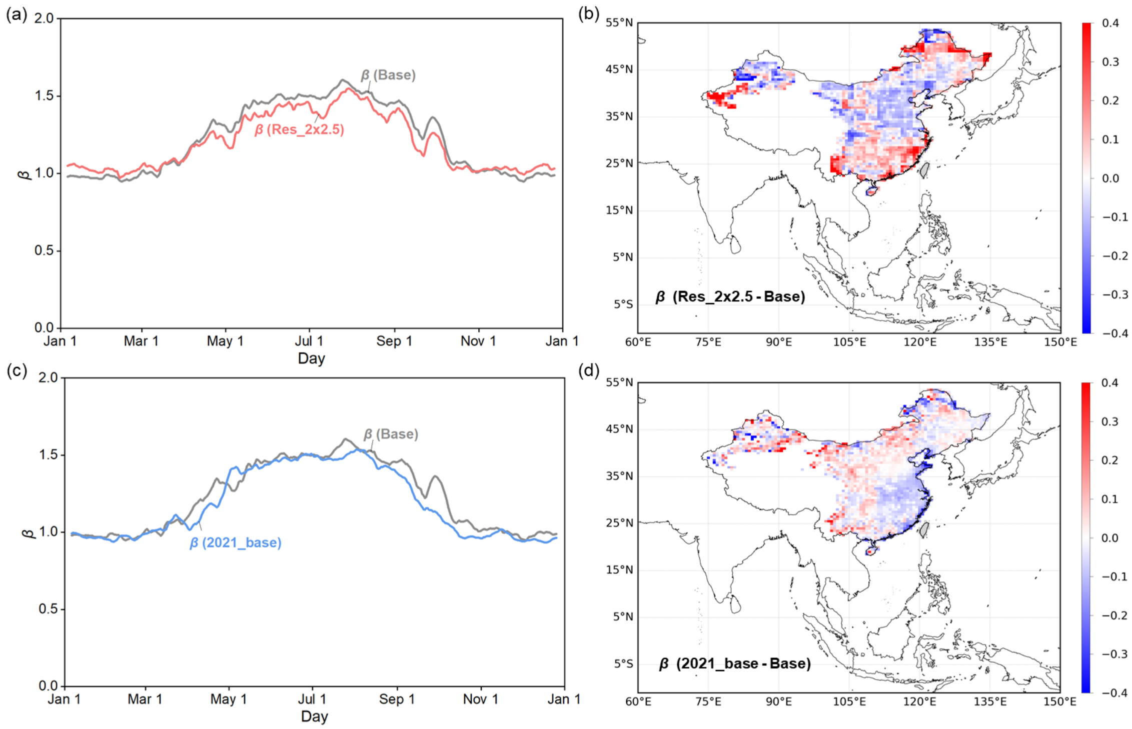

Figure S8. **Comparison of *β* between Res_2×2.5 and Base, 2021_base and Base.** (**a**) and (**c**) compare the daily *β* dynamics between Res_2×2.5 and Base, and between 2021_base and Base, respectively. (**b**) and (**d**) present the spatial distribution of *β* variance between Res_2×2.5 and Base, and between 2021_base and Base, respectively. The gray shaded area is not calculated in this study.

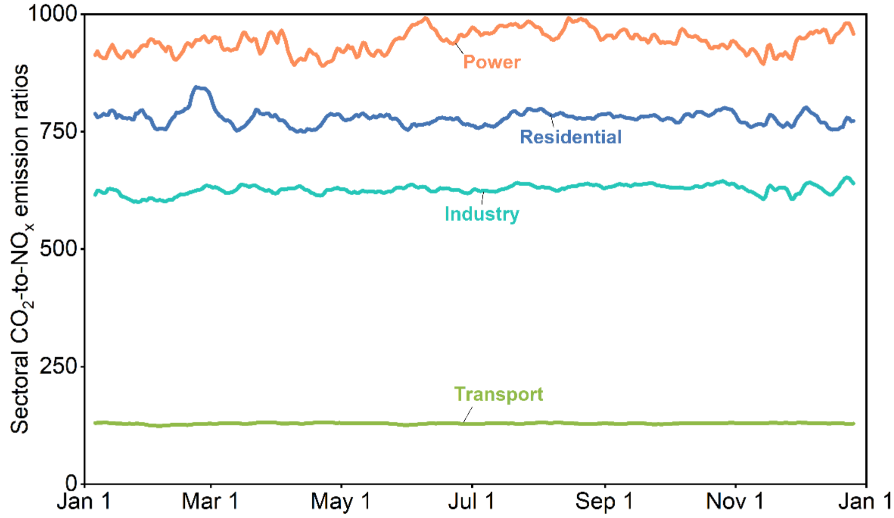

Figure S9. **Sectoral CO_2-to-NO_x emission ratios in 2022 under Base inversion.** Sectors are color coded.

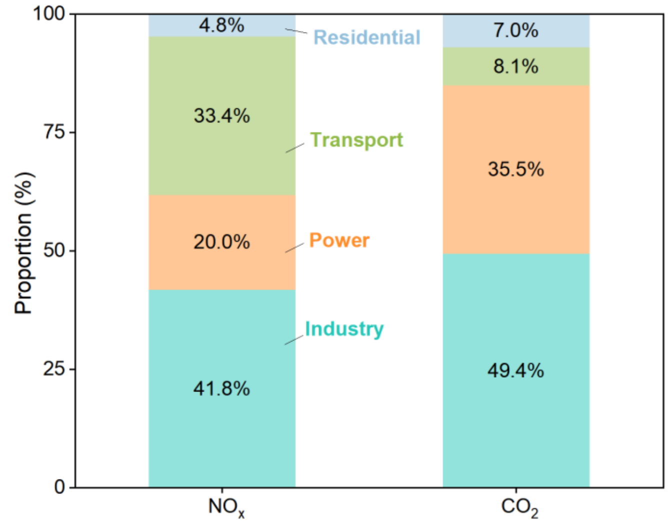

Figure S10. Sectoral contribution to total NO_x and CO_2 emissions in 2022 under Base inversion. Sectors are color coded.

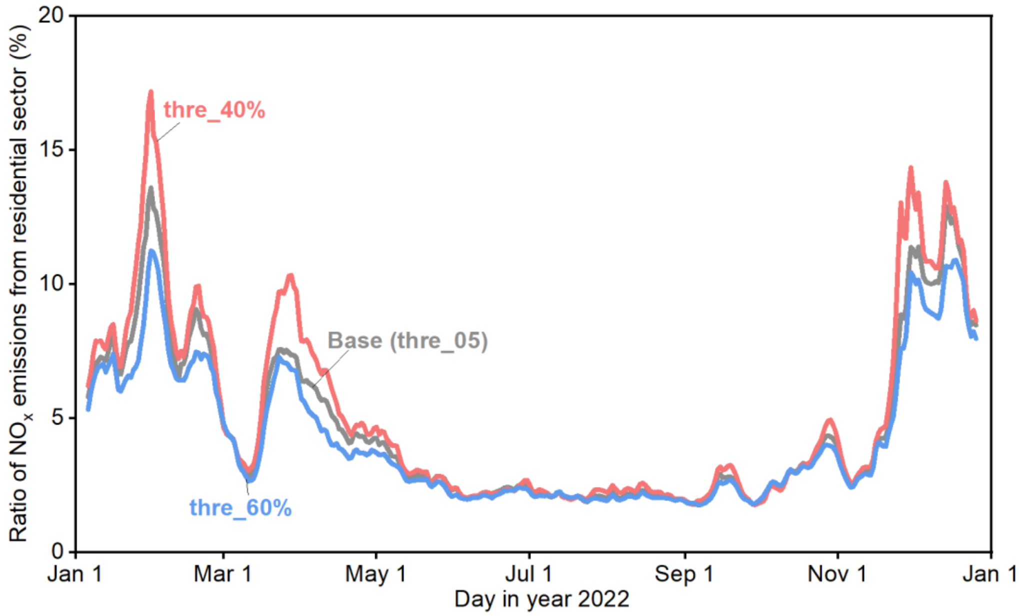

Figure S11. **The comparison of proportion attributing total TROPOMI-constrained NO_x emissions to the residential sector.** Black, red, and blue lines refer to the Base, thre_40% and thre_60% inversions, respectively.

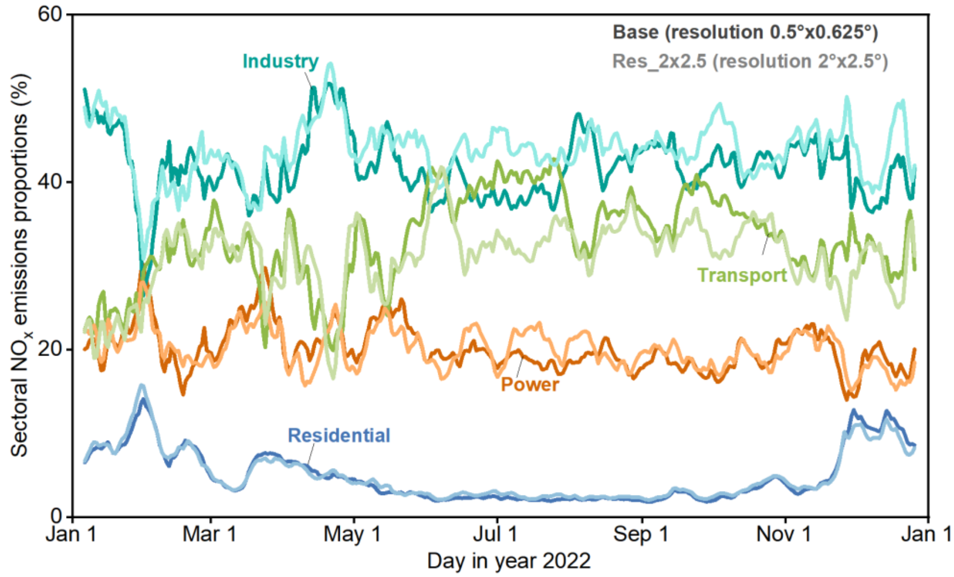

Figure S12. **The comparison of sectoral proportion of TROPOMI-constrained NO_x emissions.** Sectors are color coded. Deep color refers to the Base inversion, and light color represents the Res_2×2.5.

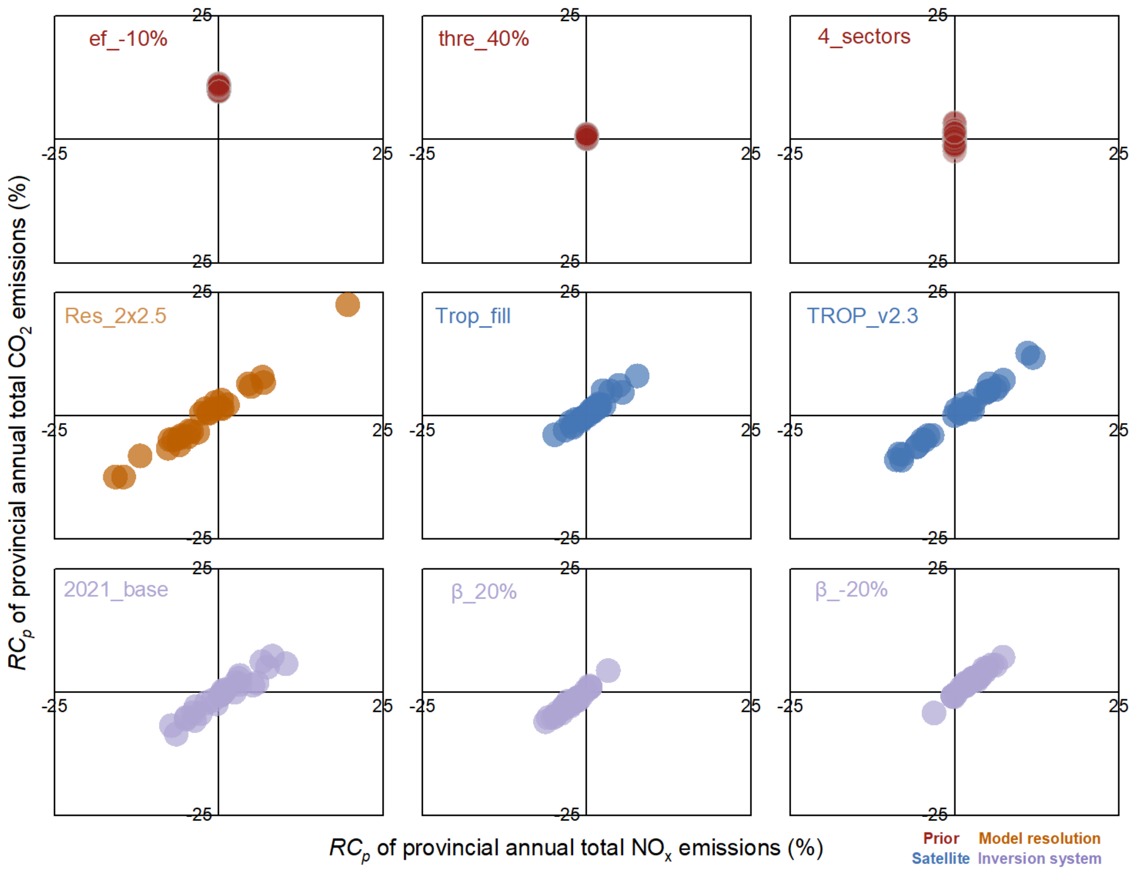

Figure S13. Correlation between RC_p in provincial annual total NO_x and CO_2 emissions. Scatters in red, orange, blue, and purple colors show the results from the tests on prior, model resolution, satellite retrievals, and inversion system parameters, respectively.

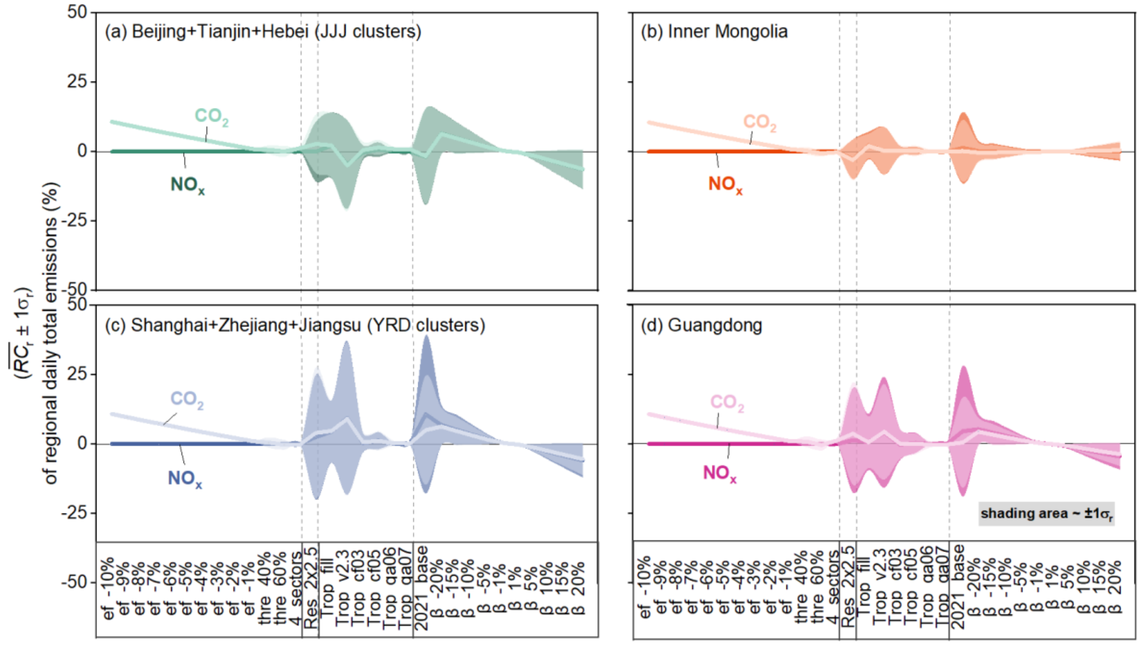

Figure S14. Response of regional total NO_x and CO_2 emissions under tests on a daily scale. (**a**), (**b**), (**c**), and (**d**) show the $\overline{RC_r} \pm 1\sigma_r$ of daily NO_x (deep color) and CO_2 (light color) emissions triggered by different tests in Jing-Jin-Ji clusters (Beijing, Tianjin, and Hebei), Inner Mongolia, Yangtze River Delta clusters (Shanghai, Zhejiang, and Jiangsu), and Guangdong.

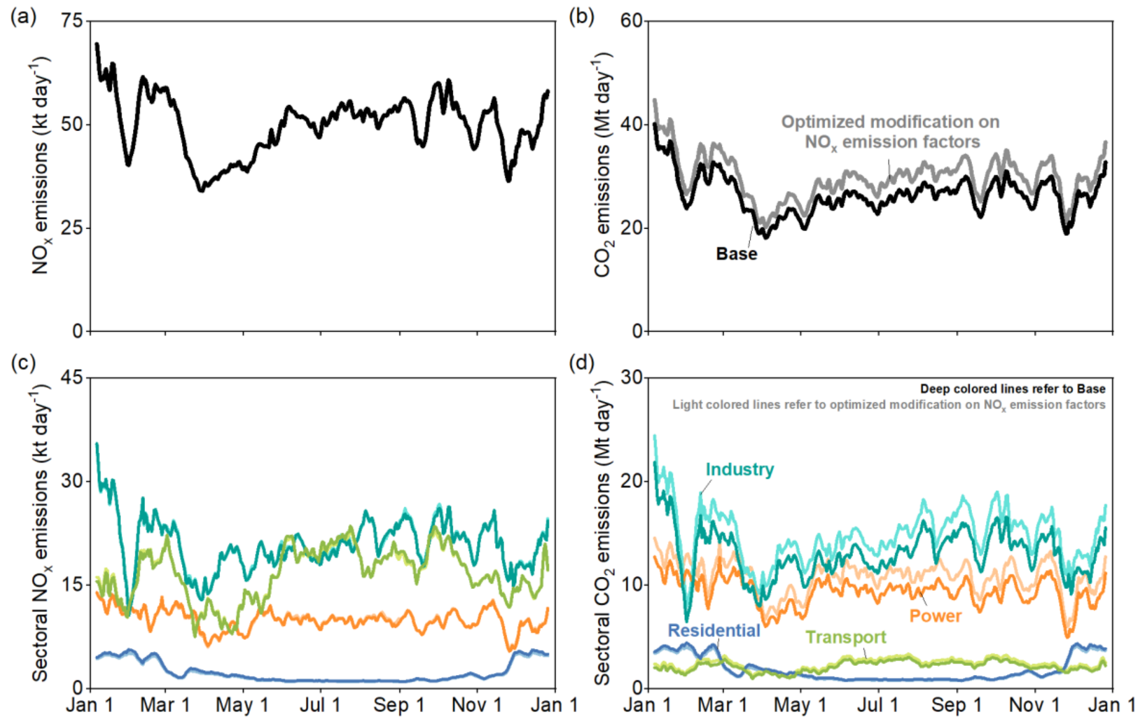

Figure S15. Comparison of daily NO_x and CO_2 emissions between Base and situation with iteratively optimized modification on NO_x emission factors. (**a**) and (**c**) present the total and sectoral NO_x emissions under Base (deep color) and situation with iteratively optimized modification on NO_x emission factors (light color). (**b**) and (**d**) are plotted for CO_2 as (**a**) and (**c**).