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Supplement of

Inversion-based assessment of anthropogenic NO_x emission changes in Ukraine during the 2022–2023 war using TROPOMI satellite data

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Supplemental Texts

S1: NO_x Emissions During the Pandemic

The inversion results reveal that the COVID-19 epidemic in 2020 exerted a more moderate and short-lived suppression effect on Ukraine's NO_x emissions compared to the impact of war. The widespread outbreak of the coronavirus disease in Ukraine in 2020 commenced in April (Malarvizhi et al., 2023) and was accompanied by a notable reduction in emissions at the end of April, followed by a significant decline in emissions observed in May. The transport sector experienced the most substantial decrease, with emissions reduced by 3.9% (±0.6%) from May to December, largely attributable to mobility restrictions imposed by public health measures. Agricultural emissions declined only slightly by 0.5%, while industrial and residential emissions increased in 2020. It can be explained by the continued operation of agriculture and industry, which were prioritized as essential sectors, and by increased domestic activities under stay-at-home guidelines, leading to elevated residential emissions.

Notably, the prior emission inventory overestimated reduction magnitudes for agricultural and transportation sectors. The posterior results indicate the actual transportat emission reduction (3.9%) was substantially lower than the prior (10%), consistent with Ukraine's relatively lenient containment measures (e.g., merely 3% decline in petroleum consumption reported by SSCU). Similarly, the posterior agricultural reduction (0.5%) was markedly smaller than the prior 9% projection, aligning with the 3.7% growth in agricultural CO_2 emissions documented by the EU Joint Research Centre. Furthermore, a 5% increase in natural gas consumption recorded by SSCU provides additional evidence supporting the posterior conclusion of rising residential emissions.

Compared to 2022, changes in NO_x emissions across Ukraine during the COVID-19 pandemic in 2020 exhibited a distinct spatial pattern, characterized by slight increases in the west and decreases in the east, although the overall east–west gradient remained modest (Figs. S12). In both eastern and western Ukraine, NO_x emission reductions across all sectors were consistently smaller than those observed in 2022. This spatial pattern can be attributed to several factors. Unlike the large-scale population displacement triggered by the war, the COVID-19 outbreak did not result in significant population movement. The imposed lockdown measures substantially reduced transportation-related emissions, while also offsetting potential reductions in agricultural and residential sectors. Notably, western

Ukraine experienced an increase in NO_x emissions compared to the baseline year, with a pronounced emission peak observed in June. This increase likely reflects a rapid rebound in industrial activity, transportation, and logistics following the easing of the first national lockdown, which began lifting after May.

Supplemental Tables

Table S1 Key updates and their potential impact on NO_2 VCD of versions v2.4.0~v2.6.0 of TROPOMI NO_2 VCDs

Version	Time period	Key updates	Potential impact on NO_2 VCD
v2.4.0	1 May 2018 – 12 Mar. 2023	Improved Air-mass factor (AMF) (surface albedo, clouds), updated cross-sections	Better consistency with validation; no major discontinuity
v2.5.0	13 Mar. – 26 Nov. 2023	Bug fix in quality assurance value (qa_value) (snow/ice handling)	Slightly more valid pixels; minimal effect on mean NO_2
v2.6.0	26 Nov. 2023 – 8 Sep. 2024	Fast Retrieval Scheme for Clouds from the Oxygen A band cloud pressure update affecting AMF	Small regional shifts in VCD (few percent); limited in our study due to short time span

Supplemental Figures

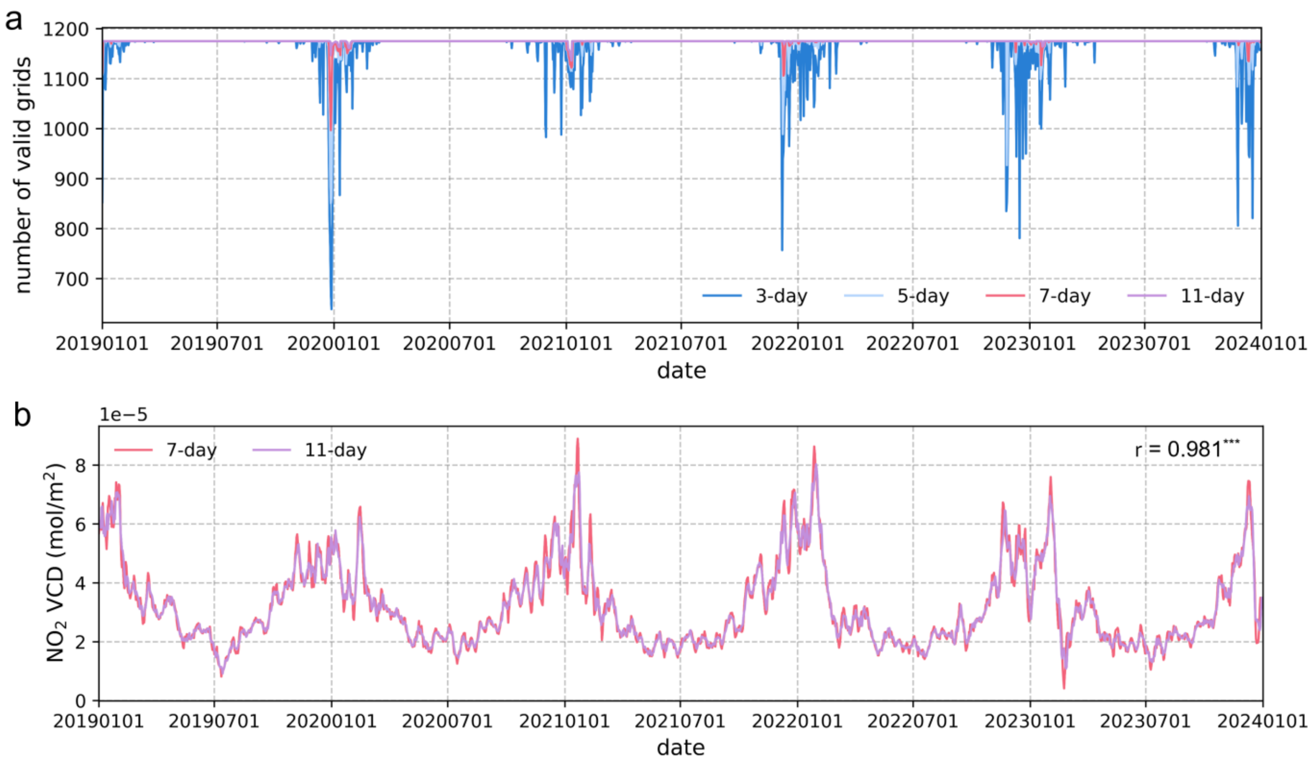

Figure S1 (a) Number of valid TROPOMI observation grids over Ukraine from 2019 to 2023 under different moving average window lengths. (b) Comparison of daily TROPOMI NO_2 VCDs over Ukraine using 7-day and 11-day moving averages.

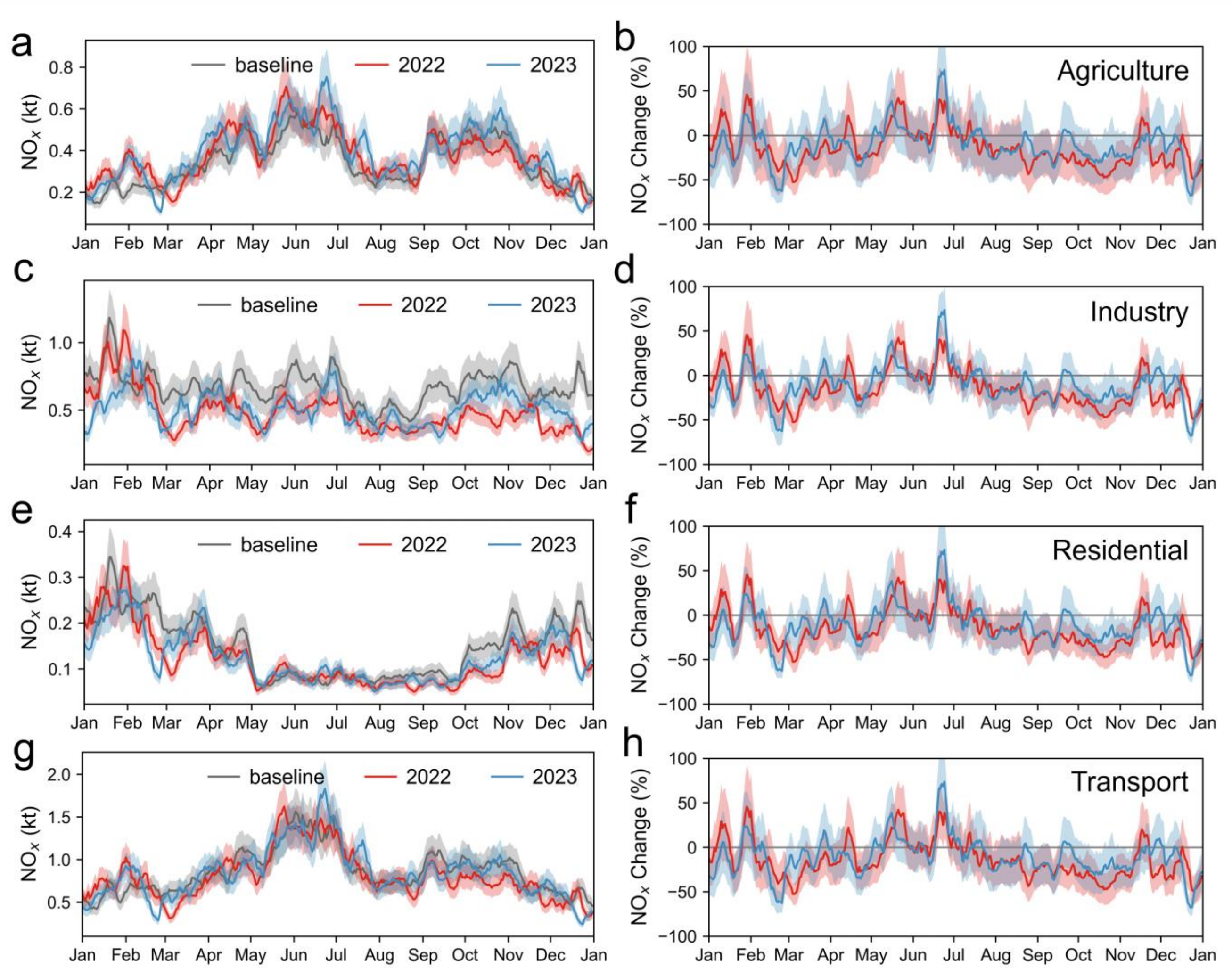

Figure S2 Seasonal changes of sectoral NO_x emissions in Ukraine in 2022, 2023 and baseline; and the relative changes of 2022 and 2023 with baseline year.

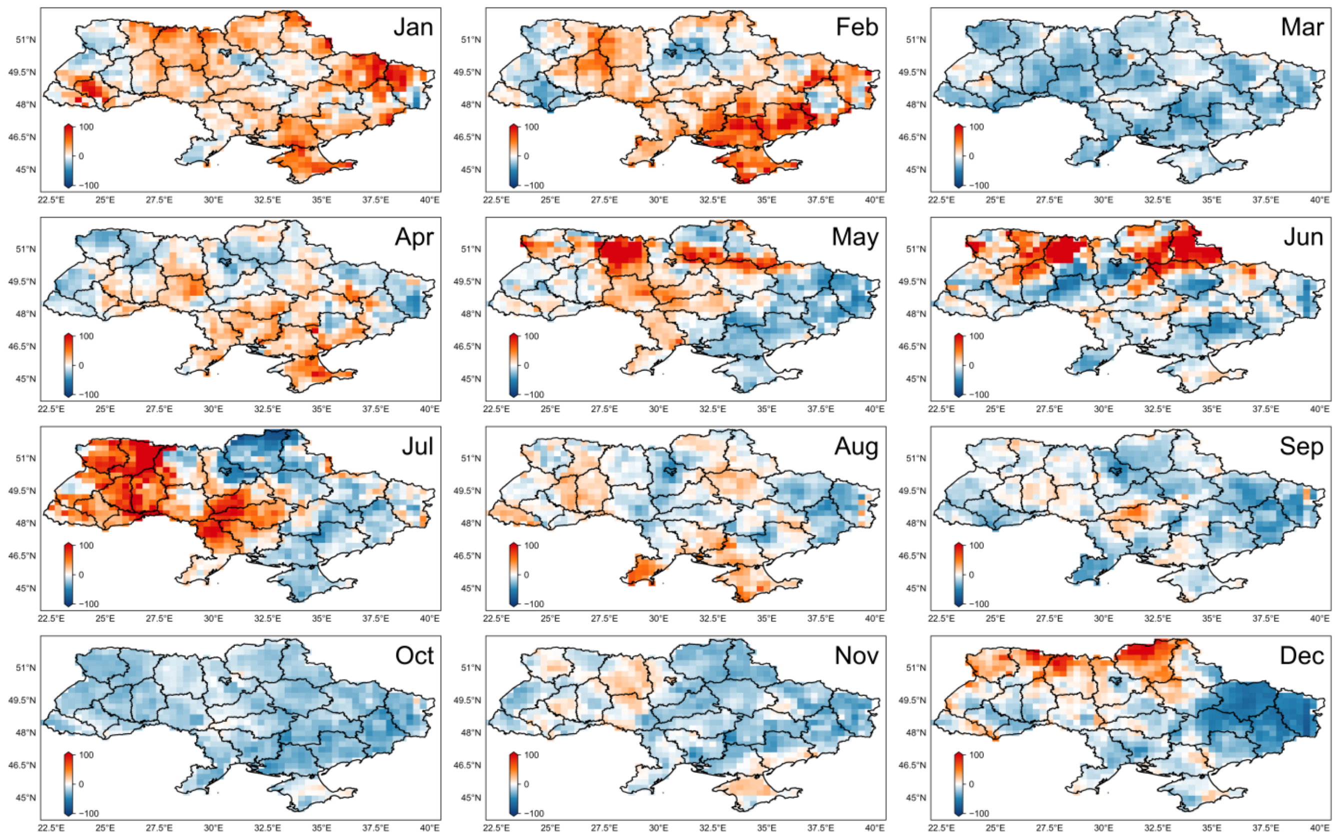

Figure S3 Spatial distribution of monthly NO_x emission changes during the war (March to December) in 2022 relative to the baseline year.

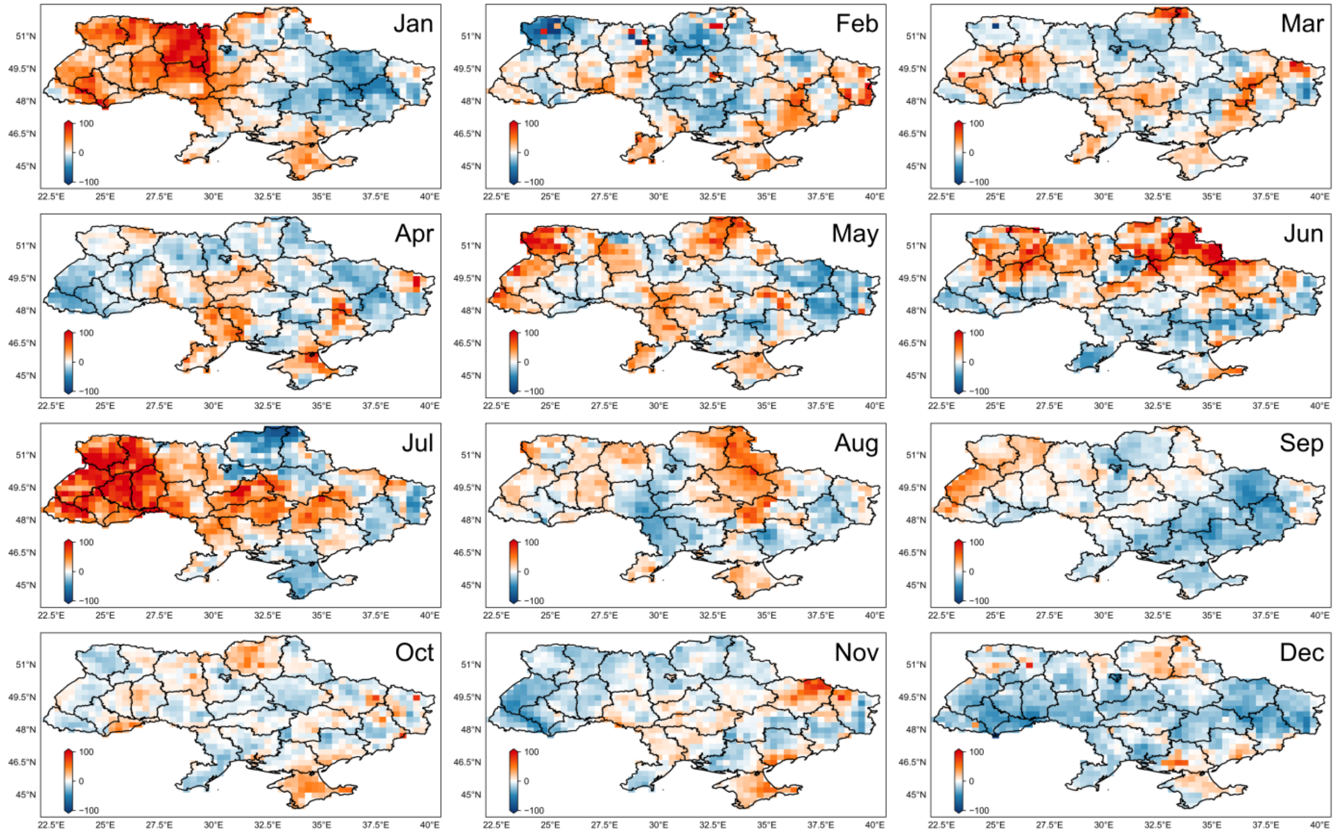

Figure S4 Spatial distribution of monthly NO_x emission changes during the war (March to December) in 2023 relative to the baseline year.

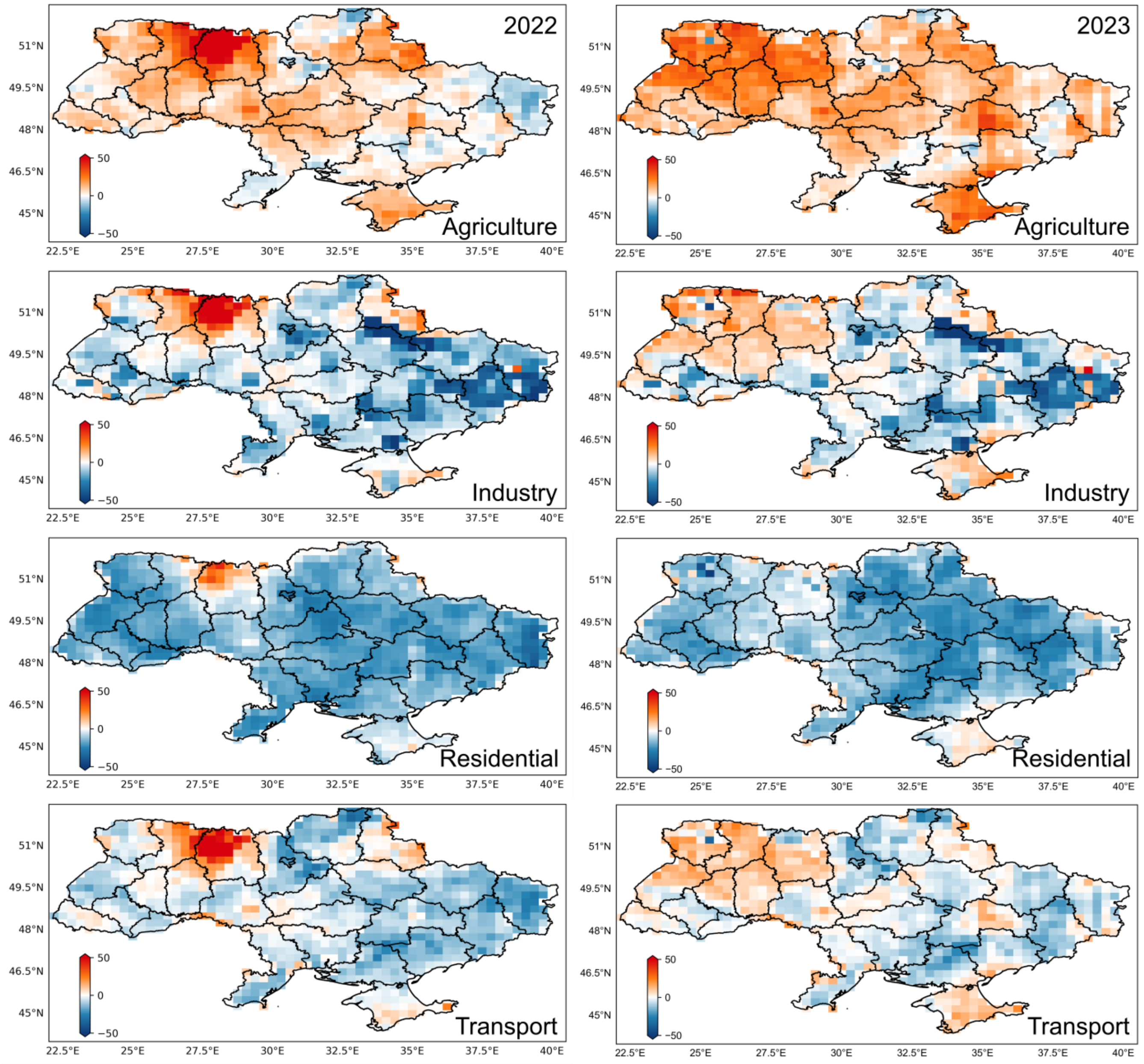

Figure S5 Spatial changes of sectoral NO_x emissions in Ukraine in 2022 and 2023 relative to the baseline year.

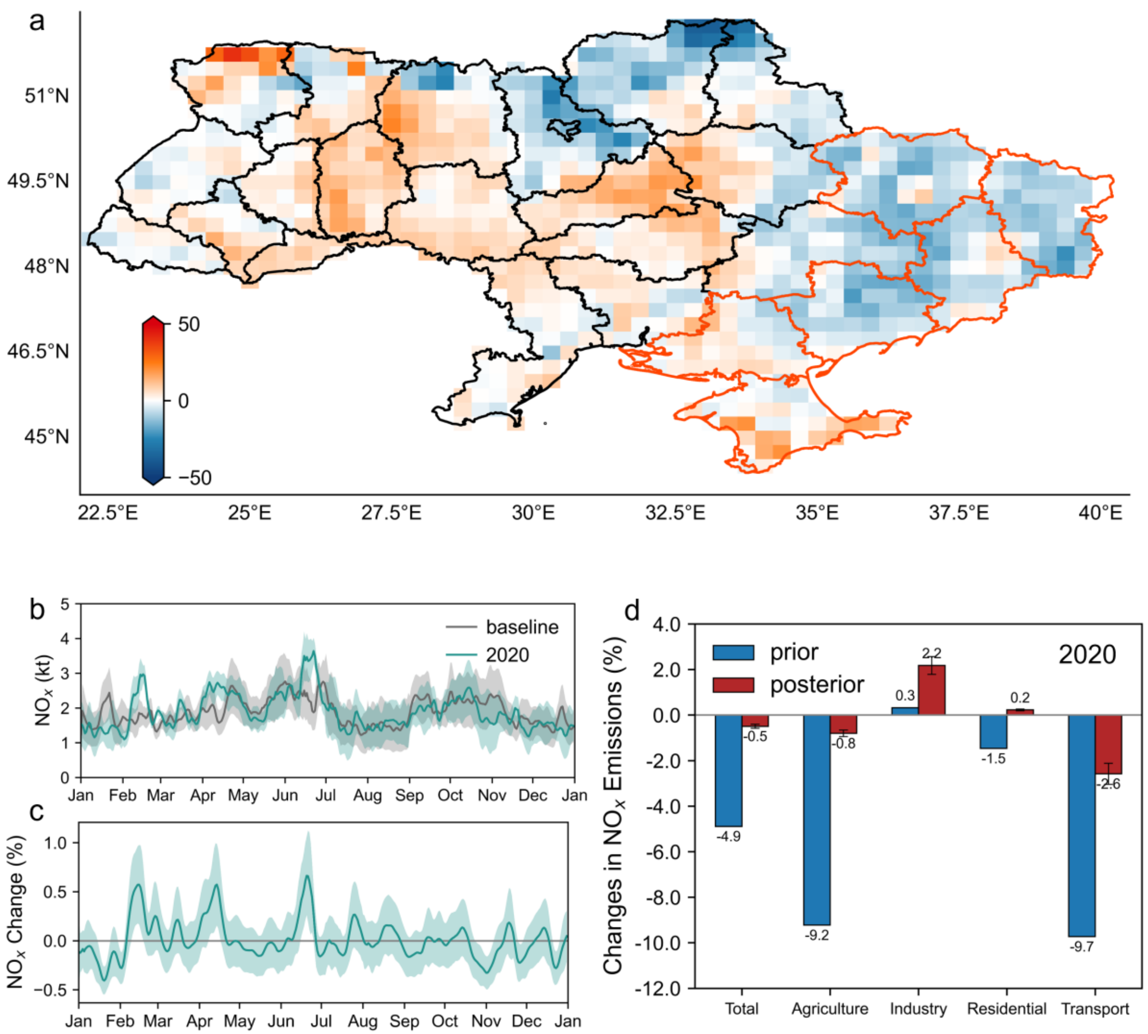

Figure S6 Seasonal and sectoral NO_x emission changes in Ukraine in 2020. (a) Spatial changes of NO_x emissions in Ukraine in 2020 relative to the baseline year. (b) Daily NO_x emissions in 2020 and the baseline year, and (c) relative changes in daily emissions in 2020 compared to the baseline year. (d) Relative changes in different sectors in 2020 compared to the baseline year.

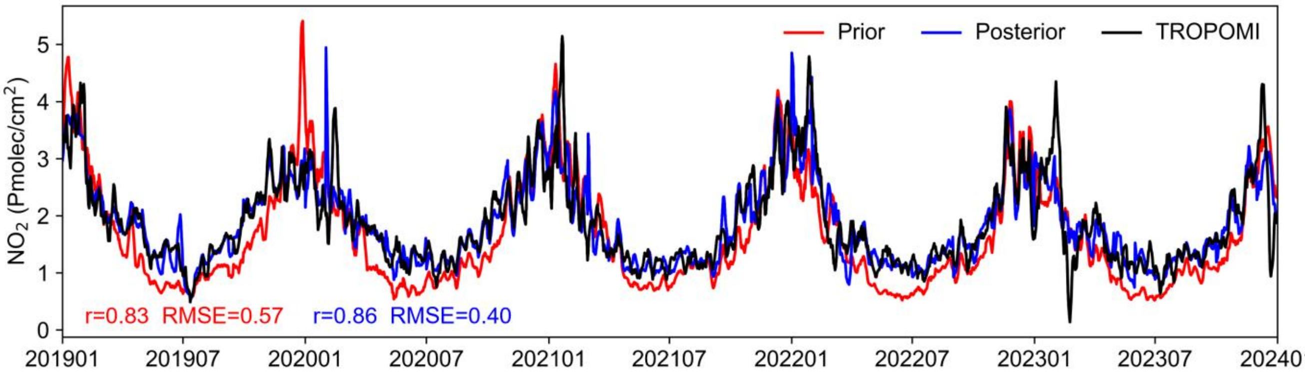

Figure S7 Daily average NO_2 VCDs estimated from the prior and posterior emission inventories versus satellite-observed NO_2 VCDs seasonal changes from 2019 to 2023.

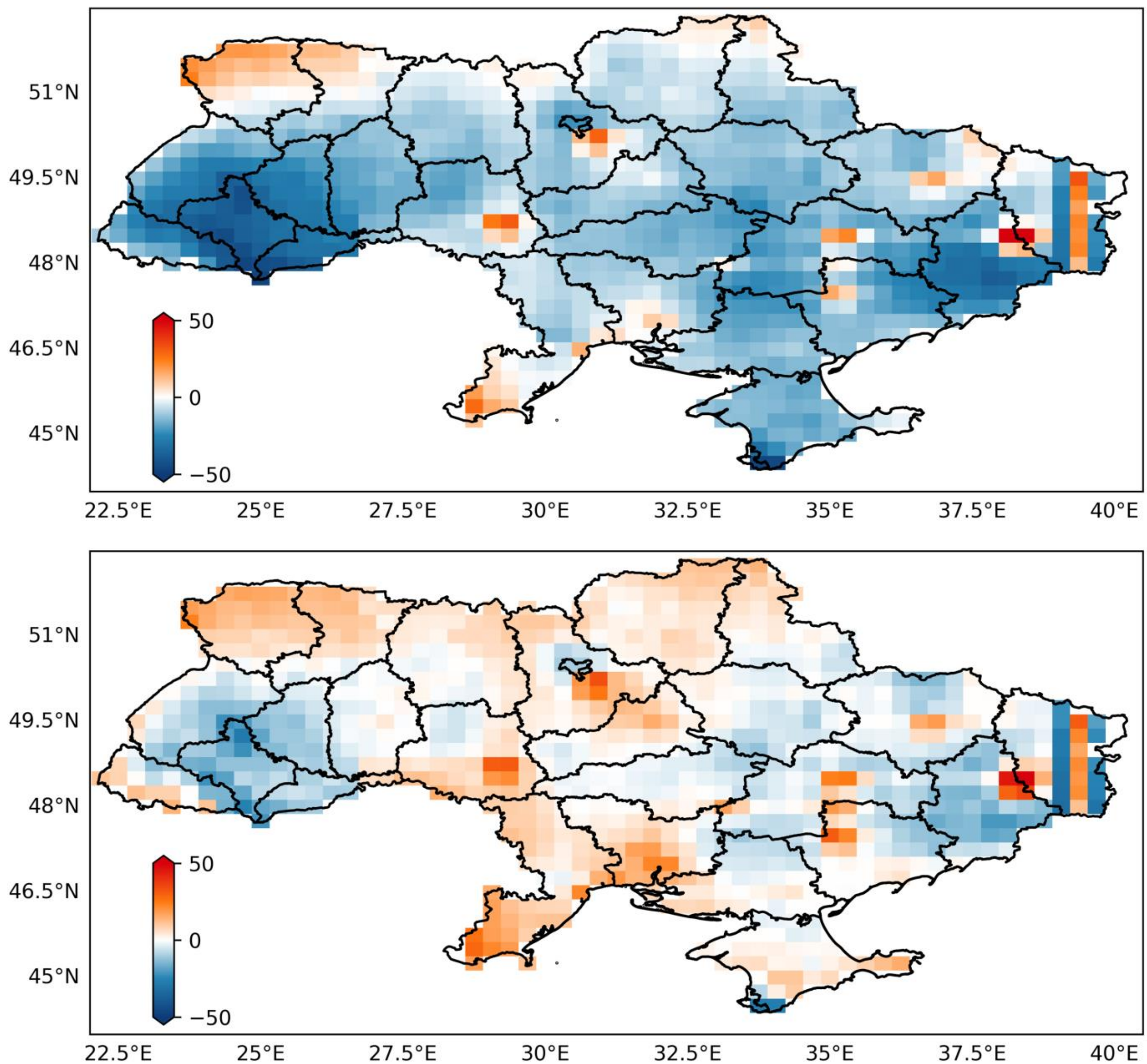

Figure S8 Spatial distribution of relative deviations between the prior emissions and inverted the posterior emissions modeled NO_2 VCDs and satellite observations.

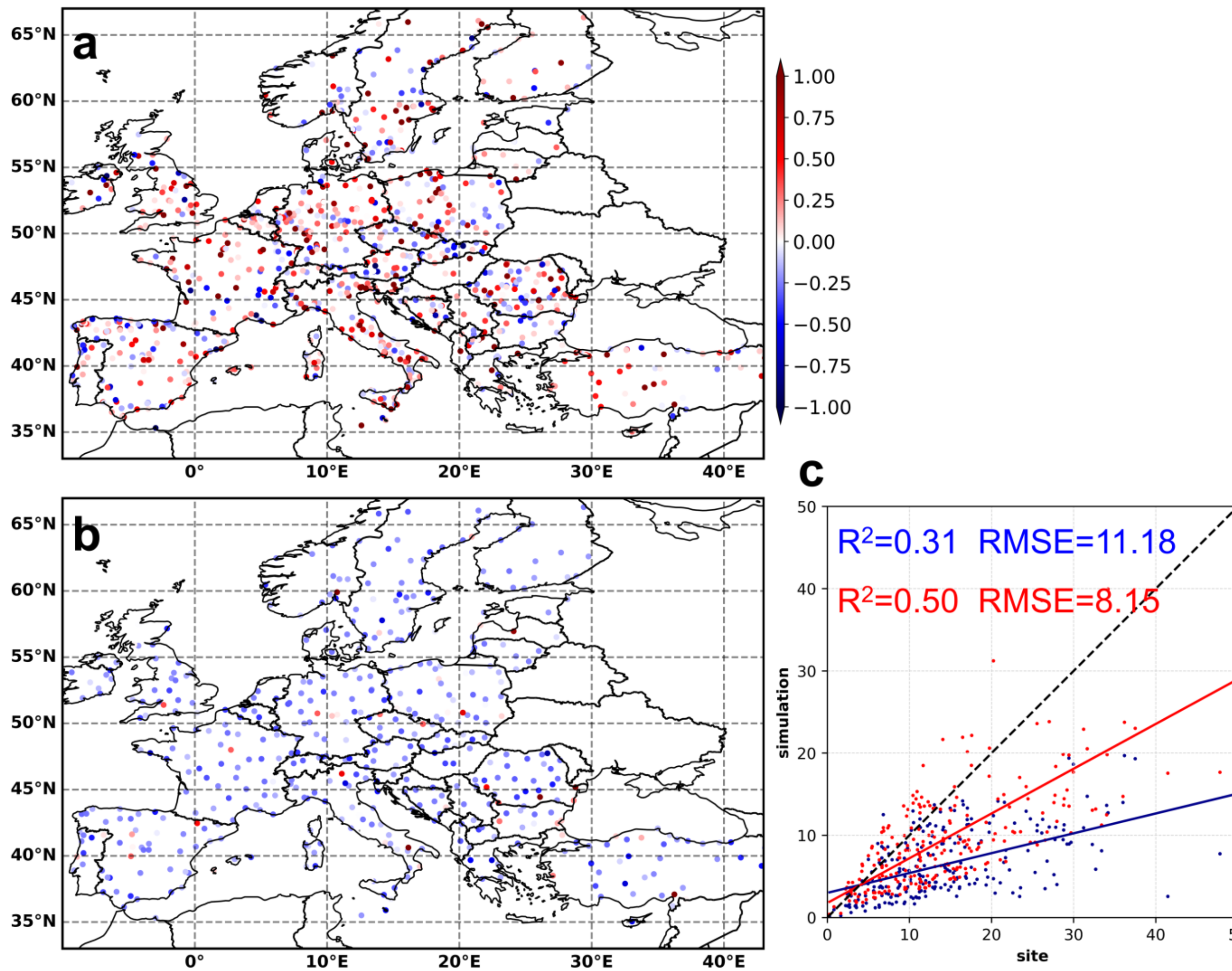

Figure S9 Accuracy of priori and posteriori emission simulated surface concentration with in-suit observations. (a) Relative change in R^2 of the time series of in-suit observations to the posterior versus prior simulated surface concentration in the corresponding grids (($R^2_{posterior}$- R^2_{prior})/R^2_{prior}); (b) Relative change in RMSE of the time series of in-suit observations to the posterior versus prior simulated surface concentration in the corresponding grids (($RMSE_{posterior}$- $RMSE_{prior}$)/$RMSE_{prior}$); (c) Scatterplot of the linear fit of the time-averaged values of in-suit observations to the priori (blue) and posterior (red) simulated concentrations of the corresponding grids.

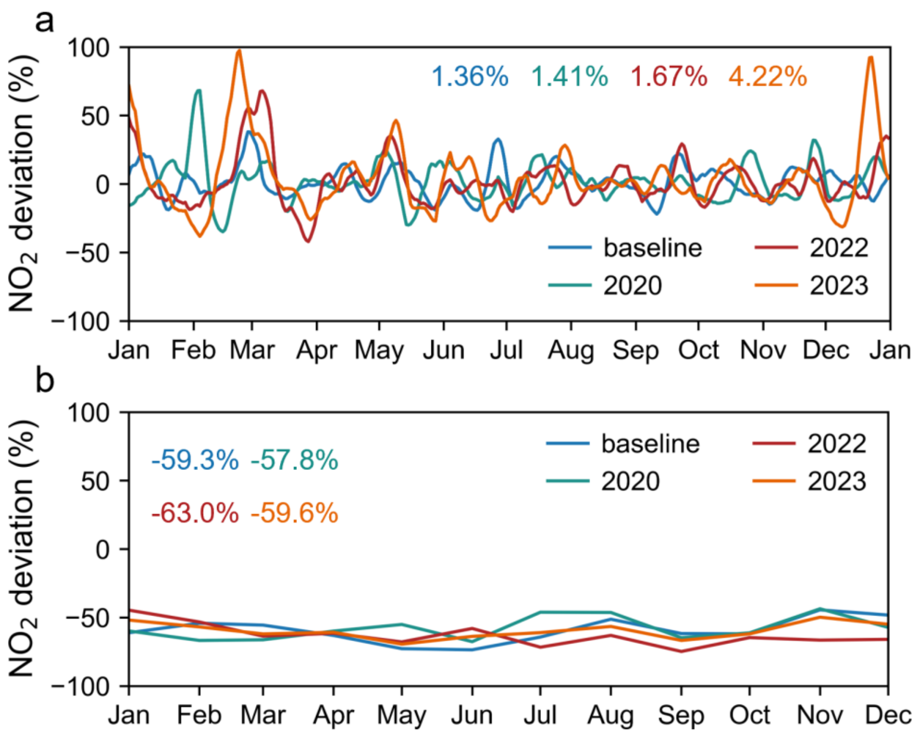

Figure S10 Seasonal distribution of the relative deviations in posterior simulations in the baseline, 2020, 2022 and 2023, with respect to (a) satellite observations and (b) surface in-suit observations.

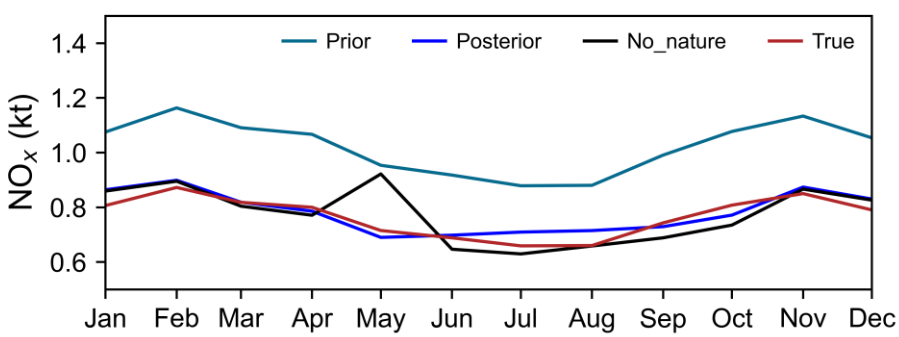

Figure S11 Seasonal changes of posterior Ukrainian anthropogenic NO_x emissions considering natural source emissions (Posterior) versus those without natural source emissions (No_nature) with pseudo-true values (True) and prior (Prior) emissions in the OSSE test in 2023.

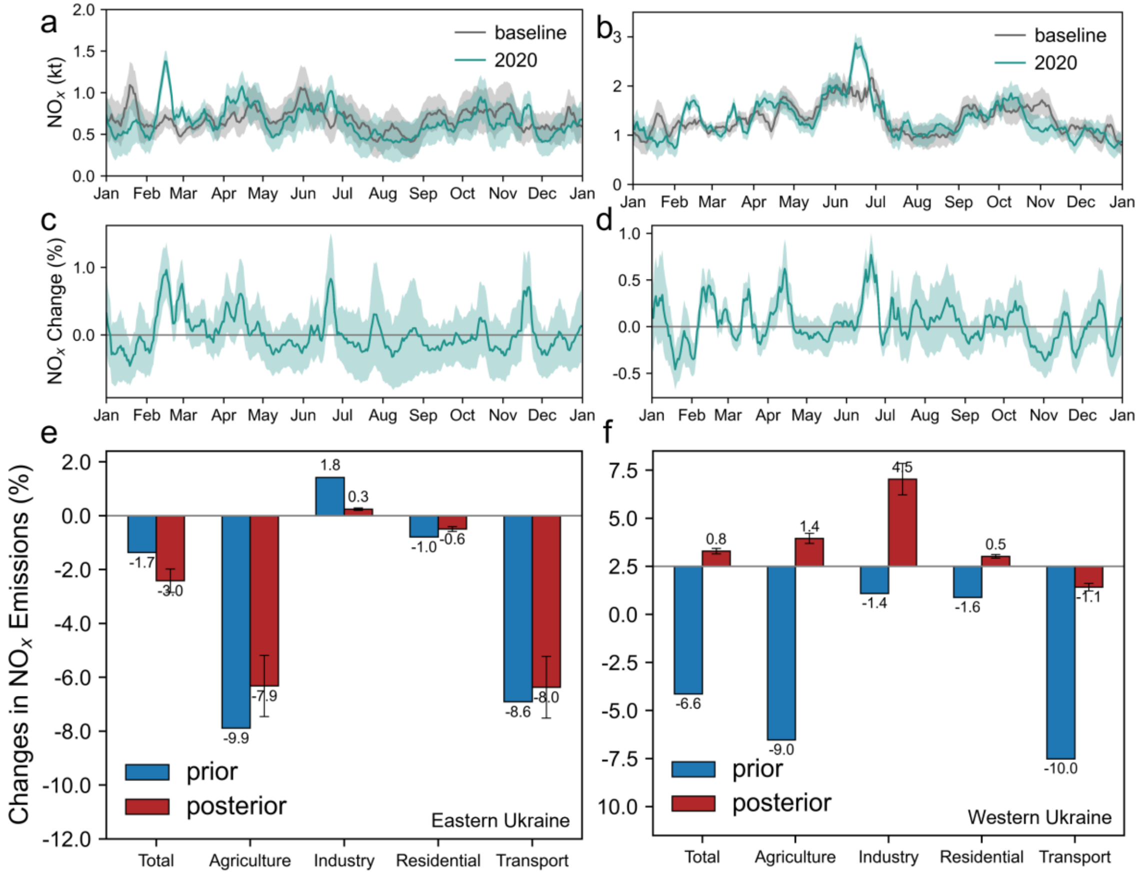

Figure S12 Seasonal and sectoral NO_x emission changes in Eastern and Western Ukraine in 2020. (a~b) Daily NO_x emissions in 2020 and the baseline year in (a) Eastern and (b) Western Ukraine. (c~d) Relative changes in daily emissions in 2020 compared to the baseline year in (c) Eastern and (d) Western Ukraine. (e~f) Relative changes in different sectors in 2020 compared to the baseline year in (e) Eastern and (f) Western Ukraine.

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