

Authors' response to referee comments #2 regarding 'An improved Bayesian inversion to estimate daily NO<sub>x</sub> emissions of Paris from TROPOMI NO<sub>2</sub> observations between 2018-2023' by Mols et al. (2025).

The reviewer's comments are in black, the authors' replies in blue

## Reviewer #2

Title: An improved Bayesian inversion to estimate daily NO<sub>x</sub> emissions of Paris from TROPOMI NO<sub>2</sub> observations between 2018-2023

Author(s): Alba Mols et al.

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### General Comments

Mols et al. introduce a Bayesian inversion method which determines urban NO<sub>x</sub> emissions at daily scale from along-wind line densities. These line densities are produced by integrating TROPOMI NO<sub>2</sub> vertical column densities in the cross-wind direction. The study first shows that a simple forward model can represent the relationship between emissions at each cell and the retrieved line densities. Then, a Bayesian approach is introduced where the inversion of this forward model with measured line densities is used to find emissions. Generally, the spatial distribution of NO<sub>2</sub> depends on both lifetime and emissions. A significant advantage of this study's approach is the incorporation of prior information on lifetime and emissions into the cost function of the inversion. These priors avoid the overestimation of emissions due to unrealistic representations of the lifetime. The above method is shown to prevent the overfitting of a simpler least-squares inversion, which overpredicted emissions compared to simulated data. The determination of NO<sub>x</sub> emissions over Paris between 2018-2023 illustrates interesting effects due to the COVID-19 lockdowns, the low-emission zone, and temperature. The differences between the findings of Lorente et al. and this study are discussed well. The idea is interesting. I recommend publication after attention to the items below.

We thank the reviewer for their insightful comments and suggestions. The points raised have contributed a lot to improving the clarity and quality of the manuscript. Please see below for replies to the specific comments.

### Major comments

- The assumption that the TROPOMI retrieval is accurate enough to support the authors' analysis should be further explored. The role of a number of resolution dependent aspects of the a priori used in retrievals that would result in systematic biases between city centers and their surroundings have been reported in the literature. It is important to note that these biases always reduce gradients

between peaks in urban plumes and their surroundings. They are not simple random uncertainties. Examples are listed in the references below.

Using low-resolution input in AMF calculations can lead to "resolution dampening," particularly when surface albedo (~50 km) and a priori NO<sub>2</sub> profiles (~100 km) are much coarser than the TROPOMI NO<sub>2</sub> pixel (~5 km). However, here we use TROPOMI v2.4, which incorporates high-resolution (0.125°) surface albedo from the DLER database (Tilstra et al., 2023) and high-resolution (0.1°) a priori NO<sub>2</sub> profiles from CAMS (Douros et al., 2021). These improvements mitigate concerns about insufficient spatial detail. For example, Lange et al. (2023) demonstrated that the v2.3 retrieval using CAMS 0.1° profiles (IUP 2.02.02.01 REG) showed strong agreement with AirMAP NO<sub>2</sub> columns in the Ruhr Area. Similar performance is expected over Paris. A corresponding clarification has been added at the end of the introduction.

Nevertheless, errors in the NO<sub>2</sub> retrieval are indeed not exclusively random. We recently investigated the issue in Rijsdijk et al. (2025) and found that there likely is a modest degree of spatial error correlation stemming from the surface albedo climatology extending over at least 2 TROPOMI pixels. We have accounted for this in Eq. (6), where we introduce an uncertainty on top of the MicroHH-simulated NO<sub>2</sub> columns. This uncertainty that we assign has a random part (originating from measurement noise) and a systematic part (accounting from AMF uncertainties). The systematic part is correlated between adjacent cells, with a Gaussian-like shape between adjacent cells with a spatial correlation length (where the correlation falls to 1/e) of 7km. We added this last clarification to the manuscript in the description of Eq. 6.

- There are many variations of the fitting approach described by Lorente et al in the literature that also aim to reduce the same biases in lifetime and emissions this paper aims to reduce. The paper should include a more complete summary of these approaches and their strengths and weaknesses relative to the stated goals. Recent papers from De Foy, et al. Liu et al, and Zhu et al. are examples, but there are many others.

We have expanded the discussion in the introduction to include a broader range of recent literature on satellite-based estimation of NO<sub>x</sub> emissions and lifetimes. However, we emphasize that the purpose of this study is not to provide a comprehensive review of existing methods, but to demonstrate and evaluate a specific, observation-driven approach. A full methodological comparison is beyond the scope of this paper.

The introduction was extended as follows: *"These methods have nonetheless been evaluated using synthetic data, with studies such as De Foy et al. (2014) and Liu et al. (2022) showing that inferred NO<sub>x</sub> emissions and lifetimes remain broadly consistent with the known model input. In a complementary approach, Zhu et al. (2022) inferred long-term changes in NO<sub>x</sub> lifetime from decadal OMI NO<sub>2</sub> observations, using machine learning to relate NO<sub>2</sub> columns to OH concentrations."*

- The paper rightly identifies correlation between NO<sub>2</sub> concentration (and emissions) and lifetime as key. It should report on trends in the lifetime with reductions in NO<sub>2</sub>. These are likely of the same magnitude as the emission reductions but are nonlinear as shown by Zhu et al. (and others). Also, the paper indicates increases in O<sub>3</sub> as an important effect on lifetime. The authors should

compare the effect of increased ozone to the effect of differences in  $\text{NO}_2$  and VOC at the two comparison points. It is likely that an increased source of OH from  $\text{O}_3$  photolysis is the smallest contributor of these effects, that VOC changes are also small and that  $\text{NO}_2$  changes dominate.

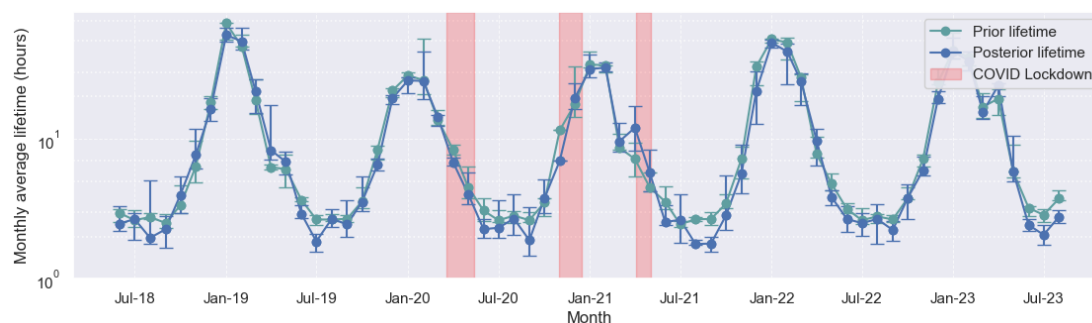
We appreciate the reviewer’s insightful comment regarding possible lifetime trends in the context of changing  $\text{NO}_x$  emissions. Our Bayesian inversion framework jointly retrieves  $\text{NO}_x$  emissions and an effective  $\text{NO}_x$  lifetime by fitting modeled  $\text{NO}_2$  line densities to satellite-observed line densities. While this setup captures broad trends, we caution against overinterpreting the retrieved lifetime values as chemically precise quantities.

As demonstrated in our end-to-end test (Table 3 and Figure 4), the lifetime retrievals are subject to significant biases --up to 30%-- highlighting the limitations of the method. This bias stems from the inherent asymmetry in the inversion sensitivity: the  $\text{NO}_2$  line density is strongly and directly influenced by the strength of the  $\text{NO}_x$  emissions, whereas the lifetime exerts a more subtle control through the dampening of the increase in line densities with distance. In practice, the signal from  $\text{NO}_x$  emissions dominates the inversion, while the  $\text{NO}_x$  lifetime estimate is more a regularization parameter that prevents overfitting than a robust diagnostic of possible changes in atmospheric chemistry.

As suggested by the reviewer, we examined trends in both prior and posterior  $\text{NO}_x$  lifetime estimates over Paris. The CAMS prior suggests a modest increase in lifetime from 2.9 hours in summer 2018 to 3.5 hours in summer 2023. In contrast, our posterior (top-down) estimates indicate relatively stable  $\text{NO}_x$  lifetimes of 2.7 hours for both summers.

This apparent stability, despite a substantial decline in  $\text{NO}_x$  emissions, is consistent with the hypothesis of a transition out of the  $\text{NO}_x$ -saturated regime, as proposed by Zhu et al. (2022) and Johnson et al. (2024). In such a regime,  $\text{NO}_x$  reductions can lead to stable or higher OH levels due to reduced titration.

However, AirParif measurements at the Eiffel Tower (~300 m altitude) show a ~20% decrease in  $\text{O}_3$  concentrations and no significant change in  $\text{NO}_x$ : $\text{NO}_2$  ratios between the Summers of 2018 and 2023. This suggests that while  $\text{NO}_x$  reductions would favor a shorter lifetime, concurrent decreases in  $\text{O}_3$  could partly counteract this by limiting OH production. The net effect on OH --and thus on  $\text{NO}_x$  lifetime-- is likely small and falls within the uncertainty bounds of our inversion framework. We now include a sub-panel in Figure 5 (shown below) showing the time series of prior and posterior  $\text{NO}_x$  lifetime estimates over Paris to illustrate this point and discuss the implications along the lines of the above text at the end of section 4.2.1.



- The reported improved performance is based on using the domain average lifetime of the simulation as the prior for the inversion. When applying to measured TROPOMI data, the prior lifetime is estimated from the average OH concentration in CAMS. However, a domain average lifetime is a poor approximation to a lifetime that is an explicit non-linear function of NO<sub>2</sub>.

We acknowledge that using a domain-average OH concentration is a simplification since the effective NO<sub>x</sub> lifetime exhibits spatial variability across an urban domain (Figure 3). However, this simplification is explicitly recognized in our framework: the CAMS-based prior is treated as an initial estimate, and we assign substantial uncertainty to it for exactly this reason. The role of the prior is to regularize the inversion, not to dictate its outcome. The posterior lifetime is ultimately constrained by the satellite NO<sub>2</sub> observations and reflects the actual spatial NO<sub>2</sub> distribution more realistically.

To better support this, we now include in Table 1 the mean and 1- $\sigma$  spread in NO<sub>x</sub> lifetimes from the high-resolution MicroHH simulations, which show about 50% spatial variation in lifetime across the domain (see also Figure 3(a) and 3(d)). This spatial spread confirms that while there is local variability, the domain-mean value remains a reasonable approximation within the context of the uncertainty assigned to the prior.

Therefore, the inversion corrects for biases in the prior, and the posterior reflects the lifetimes consistent with the observed NO<sub>2</sub> gradients, providing a robust estimate of effective NO<sub>x</sub> lifetime over the city.

- Since the prior is shown to have a significant impact on the inversion, the changing controls on lifetime should be discussed in the context of conclusions on NO<sub>x</sub> emissions during different seasons and across long-term trends.

We agree that the prior lifetime influences the inversion outcome and that the chemical controls on NO<sub>x</sub> lifetime are a factor in interpreting seasonal and long-term emission trends. As mentioned earlier, we have added a panel to Figure 5 showing the time series of both prior and posterior NO<sub>x</sub> lifetime estimates over Paris and include a discussion of their relationship.

Our inversion's sensitivity to lifetime is inherently weaker than to emissions due to the asymmetry in how these two parameters affect NO<sub>2</sub> line densities. Emissions influence the absolute magnitude of the column, while the lifetime modulates the downwind gradient more subtly. Our discussion emphasizes that the inversion consistently retrieves shorter posterior lifetimes than the CAMS prior in summer months, and lower posterior emissions year-round. The fact that both quantities decrease relative to the prior strengthens the conclusion of a real and substantial decline in NO<sub>x</sub> pollution over Paris from 2018 to 2023. Thus, the seasonal pattern in the posterior relative to the prior provides meaningful insight: the inversion's outcome is consistent with a chemically evolving atmosphere in which reduced NO<sub>x</sub> emissions contribute both directly and indirectly to observed NO<sub>2</sub> concentration trends.

## Specific Comments

**Line 43:** Other methods of simultaneous lifetime/emission derivation have been demonstrated and evaluated with satellite measured NO<sub>2</sub> columns. A more comprehensive summary of the literature and prior analysis is needed here.

We added the below text to the introduction to better discuss other methods:

*“Research and refinement of inversion methods for estimating NO<sub>x</sub> emissions and lifetimes are crucial, especially for initiatives like the Copernicus CO<sub>2</sub>M mission (Sierk et al., 2021), which will utilize NO<sub>2</sub> plumes to enhance CO<sub>2</sub> monitoring by more accurately pinpointing emission sources. Several studies have quantified NO<sub>x</sub> emissions based on satellite NO<sub>2</sub> retrievals by analyzing downwind plumes of NO<sub>2</sub> from large sources, using inverse modeling computations with atmospheric chemical transport models (CTMs) (e.g., Brioude et al., 2013; Cheng et al., 2021; Kurokawa et al., 2009; Krol et al., 2024; Zhu et al., 2022). However, because CTMs can present accessibility challenges and require significant computational resources, alternative methods that do not rely on CTMs have been developed and applied to estimate NO<sub>x</sub> emissions and lifetimes (e.g., de Foy et al., 2014; Beirle et al., 2011).”*

**Line 115:** The ability of the superposition forward model to accurately represent the emissions/column relationship is tested in section 2.2. Photolysis representative for Riyadh is used in the MicroHH simulation, but the application city is Paris. This is confusing. Why was this choice made? Are there any city or latitude specific aspects of the model that are not directly transferrable and affect the interpretation?

This is a fair point. Ideally, the OSSE would have been conducted under conditions representative of Paris. We used the MicroHH simulation for Riyadh primarily for practical reasons: it was already available to us and provided a realistic, urban, and polluted environment to test the superposition model on synthetic data without requiring additional computationally expensive simulations.

This is also the first time the superposition model is tested against such high-resolution synthetic observations. Our goal here is to evaluate whether the model can reproduce the relationship between NO<sub>x</sub> emissions, lifetimes, and NO<sub>2</sub> columns in a controlled but realistic setting. For that purpose, we believe the Riyadh case is suitable.

We acknowledge that differences between Riyadh and Paris, such as photolysis rates, humidity, and emission characteristics (e.g. the VOC/NO<sub>x</sub> emission ratios), can affect atmospheric chemistry and thus the details of model performance. That said, the fundamental behavior of the model should remain applicable. We also note that the winter conditions in Riyadh (case 2) may resemble summer in Paris in terms of photochemical regime, suggesting some regime overlap and comparability. While even testing the OSSE in multiple cities would have been ideal, it was beyond the scope of this study.

**Figure 1:** Add description of black arrows; are these wind vectors at different locations over Paris?

The black arrows are indeed the wind vectors at different locations. We added the following line to the caption of figure 1: “The black arrows indicate the wind speed (from the north-east)”

**Line 124:** This implies that the symmetry line densities are spaced by 5 km. In figure 3 c and f, The line densities are shown at a closer spacing of ~3 km.

We are glad that the reviewer spotted this. We indeed made the grid 10 times coarser, so the initial MicroHH resolution was 300x300m and the coarsened one is 3x3km. We corrected this in the manuscript.

**Line 186:** “We use a prior lifetime uncertainty  $s_{A,k}$  of 30%”. This uncertainty is used for the inversion of the forward model described by equations 1 and 2, where  $k$  is the chemical loss rate constant in units of inverse time. With this wording and notation, it is unclear whether  $s_{A,k}$  is referring to the uncertainty in the lifetime or in  $k$ . Since lifetime is the inverse of  $k$ , a 30% uncertainty in one value corresponds to a 233% uncertainty in the other. Further, the covariance in concentration and lifetime uncertainties is an element of the atmospheric chemistry. What are the downsides of not explicitly addressing this issue?

This is indeed the uncertainty in the lifetime of 30%, not in the decay rate. We corrected this throughout the manuscript to  $\sigma_{A,\tau}$ .

Our superposition model indeed treats lifetime as a separate parameter from emissions (and thus concentration), and assigns uncertainties to both independently. This simplifies the inversion but may neglect some nonlinearities or feedbacks that exist in the real atmosphere. Nevertheless, the simplification keeps our inversion framework manageable and remains appropriate for the spatial and temporal scales considered here. Also, the assigned uncertainties in emissions and lifetime implicitly capture part of this variability, and sensitivity tests confirm the robustness of our results to this assumption.

**Line 198:** Comment on how appropriate it is to treat the systematic uncertainty in the AMF error as random uncertainty used to draw from a normal distribution. At pixels with high emissions, the AMF error generally leads to VCDs that are biased low. This could lead to improper fitting of forward model parameters at those pixels.

Please see our response on the first major comment.

**Line 235:** Recommended to be reworded. To some readers, this may imply that the TROPOMI V2.4.0 product uses CAMS  $\text{NO}_2$  profiles even though it uses profiles from TM5-MP at  $1^\circ \times 1^\circ$ . Emphasize that the product used is the European product described in Douros et al. with  $0.1^\circ \times 0.1^\circ$  resolution profiles.

We agree and reworded this paragraph to:  
“We use the European TROPOMI  $\text{NO}_2$  product that uses CAMS a priori  $\text{NO}_2$  profiles in the air mass factor and averaging kernel calculation. This product is based on the operational TROPOMI  $\text{NO}_2$  (v2.4.0) version, and is described in Douros et al. (2022).”

**Line 238:** More context could be provided for the correction of TROPOMI bias. What was the existing TROPOMI bias at emission hotspots, and how much of this is corrected for with the 30% increase?



We included some more details on the TROPOMI bias, as described by Douros et al. (2022):

*“Douros et al. (2022) compared the standard and European TROPOMI NO<sub>2</sub> products with nine MAX-DOAS instruments, finding an average bias of –31% for the standard product and –19% for the European version. The European product reduces the bias by 5–18% at most stations and yields up to 30% higher NO<sub>2</sub> columns in emission hotspots, especially in winter. This supports its use for NO<sub>x</sub> emission estimates. We note that a bias is not necessarily a TROPOMI concern: a persistent low bias over urban areas may also stem from representativity differences: ground-based instruments sample narrow, localized air masses, while the TROPOMI pixel averages NO<sub>2</sub> over a larger and more heterogeneous area, often smoothing out urban pollution peaks.”*

**Line 288:** See general comments; this is an area where more discussion of using CAMS OH for this purpose is warranted.

The CAMS 0.4° forecast product is part of the Copernicus Atmosphere Monitoring Service and provides global 5-day forecasts of atmospheric composition at approximately 0.4° (~40 km) resolution. It includes key chemical species such as NO<sub>x</sub>, NO<sub>2</sub>, O<sub>3</sub>, CO, and OH, among others. Using CAMS OH and NO<sub>x</sub>/NO<sub>2</sub> ratios as priors in our Bayesian inversion is justified by their physical coherence, spatiotemporal completeness, and compatibility with the scale of the rotated line densities and superposition column model, which requires one single effective NO<sub>x</sub> lifetime. We now include this discussion as requested.

**Line 293:** Expand on the justification of using a 30% uncertainty for the prior lifetime when the common value is 50%. The current explanation is that 30% encompasses most of the expected 50% uncertainty, but is the 50% uncertainty not also a type of standard deviation? If not, then clarify this.

The section that the reviewer is referring to is this: *“To incorporate the uncertainty in OH concentrations and its impact on the NO<sub>x</sub> lifetimes, we choose a standard deviation of 30% on the prior lifetime ( $\sigma_{a,k}$ ) This selection aligns with the typical range of uncertainty observed in NO<sub>x</sub> lifetimes, which commonly falls within 50% (Lorente et al., 2019). By adopting a standard deviation of 30%, we encompass the majority of uncertainties within the expected 50% range, while also allowing for larger deviations in exceptional cases.”*

We clarify why we choose the value of 30%: The previous study by Lorente et al. (2019) that we are referring to here, uses the 50% uncertainty on the NO<sub>x</sub> lifetimes as a strict cut off. In their method of fitting the superposition column model, the lifetime can not vary by more than 50%. In our study, we use a prior lifetime uncertainty ( $\sigma_{a,k}$ ) of 30%, meaning that 95% (two standard deviations) of the lifetimes will fall within a 60% uncertainty, so our Bayesian cost function allows for slightly more deviation from the prior than in Lorente et al. (2019), as long as this improves the fit enough.

**Table 4 caption:** The standard deviation of the posterior is estimated using a specific date in the summer. Were other dates tested? The prescribed uncertainties may be expected to change throughout the year, such as during winter when the NO<sub>x</sub> lifetime is longer and its absolute uncertainty increases.

The reviewer raises a good point, and we agree that using only a single date is not very representative. As suggested, we repeated the same Monte Carlo test (50 runs) for 8 different dates throughout 2022. The results are shown in the table below.

		Stdev emissions (% deviation from mean)	Stdev lifetime (% deviation from mean)
Current	16/06/2023	15%	13%
Feb 2022	05/02/2022	2.0%	1.9%
	26/02/2022	0.3%	1.6%
Apr 2022	11/04/2022	11%	4.0%
	22/04/2022	10%	4.5%
Jul 2022	04/07/2022	2.9%	2.3%
	11/07/2022	3.9%	2.3%
Oct 2022	04/10/2022	2.9%	1.9%
	25/10/2022	6.6%	3.2%
<b>Average</b>		<b>6.1%</b>	<b>3.9%</b>

We do not observe a clear seasonal trend in the posterior error across these dates. This is likely because the prescribed uncertainties on the prior lifetimes and emissions (both set to 30%) are kept constant throughout the year in our main analysis, and we applied the same approach in this Monte Carlo sensitivity test.

To make the posterior error in our manuscript more representative, we have updated Table 4 in the manuscript to show the average posterior errors across these 8 days.

## Technical Corrections

**Line 95:** Remove repeated “on”

This has been corrected.

**Line 115:** Change “Riaydh” to “Riyadh”

This has been corrected.

**Figure 3 caption:** Should be “symcity” instead of “simcity” for consistency?

This has been corrected.

**Table 1:** Add units to column “Total E<sub>NOx</sub>”

Units have been added.

**Line 275:** Should this be “never completely *increased* to their original levels”?

Indeed, this has been corrected.

## References reviewer



Beirle and T. Wagner, “A new method for estimating megacity NO<sub>x</sub> emissions and lifetimes from satellite observations,” *Atmospheric Meas. Tech.*, vol. 17, no. 11, pp. 3439–3453, Jun. 2024, doi: 10.5194/amt-17-3439-2024.

Benjamin de Foy, Joseph L. Wilkins, Zifeng Lu, David G. Streets, Bryan N. Duncan, Model evaluation of methods for estimating surface emissions and chemical lifetimes from satellite data, *Atmospheric Environment*, Volume 98, 2014, Pages 66-77, <https://doi.org/10.1016/j.atmosenv.2014.08.051>.

J.H. G. M. Van Geffen, H. J. Eskes, K. F. Boersma, and J. P. Veefkind, “TROPOMI ATBD of the total and tropospheric NO<sub>2</sub> data products,” no. 2.4.0, Jul. 2022, [Online]. Available: <https://sentinel.esa.int/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-NO2-data-products.pdf>

J.L. Laughner, Zhu, Q., and Cohen, R. C., Evaluation of version 3.0B of the BEHR OMI NO<sub>2</sub> product, *Atmos. Meas. Tech.*, 12, 129-146, <https://doi.org/10.5194/amt-12-129-2019>, 2019

J.L. Laughner, A.H. Zare and R.C. Cohen, Effects of daily meteorology on the interpretation of space-based remote sensing of NO<sub>2</sub> *Atmos. Chem. Phys.* 16, 15247-15264, doi:10.5194/acp-16-15247-2016, 2016.

J.L. Laughner and R. C. Cohen, “Direct observation of changing NO<sub>x</sub> lifetime in North American cities,” *Science*, vol. 366, no. 6466, pp. 723–727, Nov. 2019, doi: 10.1126/science.aax6832.

Liu, F., Tao, Z., Beirle, S., Joiner, J., Yoshida, Y., Smith, S. J., Knowland, K. E., and Wagner, T.: A new method for inferring city emissions and lifetimes of nitrogen oxides from high-resolution nitrogen dioxide observations: a model study, *Atmos. Chem. Phys.*, 22, 1333–1349, <https://doi.org/10.5194/acp-22-1333-2022>, 2022.

Jin, Q. Zhu, and R. C. Cohen, “Direct estimates of biomass burning NO<sub>x</sub> emissions and lifetimes using daily observations from TROPOMI,” *Atmospheric Chem. Phys.*, vol. 21, no. 20, pp. 15569–15587, Oct. 2021, doi: 10.5194/acp-21-15569-2021.

Zhu, J.L. Laughner, and R.C. Cohen, Estimate of OH Trends over One Decade in North American Cities, *Proc. Nat. Acad. Sci.* 10.1073/pnas.2117399119, 2022.

## References author reply

Beirle, S., Boersma, K. F., Platt, U., Lawrence, M. G., & Wagner, T. (2011). Megacity emissions and lifetimes of nitrogen oxides probed from space. *Science*, 333(6050), 1737-1739.

Benjamin de Foy, Joseph L. Wilkins, Zifeng Lu, David G. Streets, Bryan N. Duncan, Model evaluation of methods for estimating surface emissions and chemical lifetimes from satellite data, *Atmospheric Environment*, Volume 98, 2014, Pages 66-77, <https://doi.org/10.1016/j.atmosenv.2014.08.051>.

Brioude, J., Angevine, W. M., Ahmadov, R., Kim, S. W., Evan, S., McKeen, S. A., ... & Trainer, M. (2013). Top-down estimate of surface flux in the Los Angeles Basin using a mesoscale

inverse modeling technique: assessing anthropogenic emissions of CO, NO<sub>x</sub> and CO<sub>2</sub> and their impacts. *Atmospheric Chemistry and Physics*, 13(7), 3661-3677.

Cheng, X., Hao, Z., Zang, Z., Liu, Z., Xu, X., Wang, S., ... & Ma, X. (2021). A new inverse modeling approach for emission sources based on the DDM-3D and 3DVAR techniques: an application to air quality forecasts in the Beijing–Tianjin–Hebei region. *Atmospheric Chemistry and Physics*, 21(18), 13747-13761.

Douros, J., Eskes, H., van Geffen, J., Boersma, K. F., Compernelle, S., Pinardi, G., ... & Veefkind, P. (2023). Comparing Sentinel-5P TROPOMI NO<sub>2</sub> column observations with the CAMS regional air quality ensemble. *Geoscientific Model Development*, 16(2), 509-534.

Johnson, M. S., Philip, S., Meech, S., Kumar, R., Sorek-Hamer, M., Shiga, Y. P., & Jung, J. (2024). Insights into the long-term (2005–2021) spatiotemporal evolution of summer ozone production sensitivity in the Northern Hemisphere derived with the Ozone Monitoring Instrument (OMI). *Atmospheric Chemistry and Physics*, 24(18), 10363-10384.

Krol, M., van Stratum, B., Anglou, I., & Boersma, K. F. (2024). Estimating NO<sub>x</sub> emissions of stack plumes using a high-resolution atmospheric chemistry model and satellite-derived NO<sub>2</sub> columns. *EGUsphere*, 2024, 1-32.

Kurokawa, J. I., Yumimoto, K., Uno, I., & Ohara, T. (2009). Adjoint inverse modeling of NO<sub>x</sub> emissions over eastern China using satellite observations of NO<sub>2</sub> vertical column densities. *Atmospheric Environment*, 43(11), 1878-1887.

Lange, K., Richter, A., Schönhardt, A., Meier, A. C., Bösch, T., Seyler, A., ... & Burrows, J. P. (2023). Validation of Sentinel-5P TROPOMI tropospheric NO<sub>2</sub> products by comparison with NO<sub>2</sub> measurements from airborne imaging DOAS, ground-based stationary DOAS, and mobile car DOAS measurements during the S5P-VAL-DE-Ruhr campaign. *Atmospheric Measurement Techniques*, 16(5), 1357-1389.

Liu, F., Tao, Z., Beirle, S., Joiner, J., Yoshida, Y., Smith, S. J., Knowland, K. E., and Wagner, T.: A new method for inferring city emissions and lifetimes of nitrogen oxides from high-resolution nitrogen dioxide observations: a model study, *Atmos. Chem. Phys.*, 22, 1333–1349, <https://doi.org/10.5194/acp-22-1333-2022>, 2022.

Rijsdijk, P., Eskes, H., Dingemans, A., Boersma, K. F., Sekiya, T., Miyazaki, K., & Houweling, S. (2025). Quantifying uncertainties in satellite NO<sub>2</sub> superobservations for data assimilation and model evaluation. *Geoscientific Model Development*, 18(2), 483-509.

Sierk, B., Fernandez, V., Bézy, J. L., Meijer, Y., Durand, Y., Courrèges-Lacoste, G. B., ... & te Hennepe, F. (2021, June). The Copernicus CO<sub>2</sub>M mission for monitoring anthropogenic carbon dioxide emissions from space. In *International conference on space optics—ICSO 2020* (Vol. 11852, pp. 1563-1580). SPIE.

Tilstra, L. G., de Graaf, M., Trees, V., Litvinov, P., Dubovik, O., & Stammes, P. (2023). A directional surface reflectance climatology determined from TROPOMI observations. *Atmospheric Measurement Techniques Discussions*, 2023, 1-29.

Zhu, J.L. Laughner, and R.C. Cohen, Estimate of OH Trends over One Decade in North American Cities, *Proc. Nat. Acad. Sci.* 10.1073/pnas.2117399119, 2022.