Response to Reviewer #1

We thank the reviewer for the careful evaluation of our manuscript and for the constructive comments and suggestions. Our point-by-point responses are provided below, with reviewer comments shown in blue and our replies in black.

This paper presents a thorough update on previous work, highlighting several important improvements in the Retina algorithm. The topic is relevant, and the paper is both well-structured and clearly written. As the authors emphasize, the most significant advancement over their earlier work is the integration of satellite data into the data assimilation scheme, which apparently would only have an added value when less than 5 monitoring stations are available in a specific city.

Specific comments:

1. Since the main novelty of the presented methodology lies in the integration of satellite data (TROPOMI) for urban NO_2 modeling, a longer validation period would be highly valuable. The current one-month evaluation period may not fully capture the seasonal variability in satellite retrieval quality, atmospheric dynamics, and emissions. Statistical performance metrics may therefore exhibit seasonal dependence, potentially leading to less robust conclusions regarding the added value of satellite data.

To get a better insight in the seasonal behaviour of the Retina algorithm, we performed a processing for 2019 for three different cases:

(A) Emission optimisation based on TROPOMI only
(B) Emission optimisation based on 24 surface stations only
(C) Emission optimisation and spatial assimilation of 24 surface stations

The table below shows the validation statistics per month, based on time series of hourly simulation, averaged over the 24 stations. March 2019, indicated in bold font and evaluated in the main text, offers a reasonable approximation for the yearly performance. This table is now included in Section S7 of the Supplemental Material, and references to the algorithm's seasonal behaviour are included in Sections 3.1 and 5.

2019	Obs. (μg/m³)	Correlation			RMSE (μg/m³)			Bias (μg/m³)		
		A	B	C	A	B	C	A	B	C
January	55.6	0.760	0.788	0.908	23.7	22.2	16.3	-4.7	-0.5	-1.5
February	55.4	0.790	0.835	0.909	22.2	19.6	15.9	-4.9	-1.2	-1.6
March	**36.2**	**0.753**	**0.792**	**0.900**	**18.5**	**17.2**	**13.0**	**-2.7**	**1.1**	**-0.9**
April	27.3	0.728	0.752	0.892	15.0	14.6	11.0	-2.4	0.6	-0.8
May	22.3	0.705	0.719	0.877	13.7	13.6	10.2	-2.6	-0.1	-1.1
June	24.7	0.698	0.705	0.855	14.3	14.0	11.1	-0.4	0.5	-0.7
July	26.2	0.716	0.693	0.877	15.7	15.8	11.4	-2.1	-0.2	-0.7
August	25.9	0.777	0.795	0.901	15.9	15.1	11.8	-1.8	-0.4	-1.0

September	31.5	0.741	0.795	0.901	18.5	15.8	12.6	-0.3	-0.4	-1.3
October	41.4	0.753	0.794	0.890	19.6	17.5	14.1	-2.9	0.0	-1.1
November	27.4	0.836	0.844	0.925	12.2	11.5	8.5	-2.2	-0.0	-0.6
December	40.1	0.826	0.836	0.925	15.5	14.4	10.4	-3.1	0.1	-0.7
Average	34.5	0.757	0.779	0.897	17.1	15.9	12.2	-2.5	-0.0	-1.0

As shown in the table, NO_2 observations peak during winter months. This is due to lower mixing heights and colder temperatures (leading to stronger NO_X emissions from e.g. heating and longer atmospheric lifetimes of NO_2). During the summer months, both cases (A) and (B) show the lowest RMSE, but also show poorer correlation. This can be explained the higher ratio of the RMSE to the mean observations of NO_2 during summer.

Note that the results for case (A) in March differ slightly from those in Table 3 (where for TROPOMI-only the city-wide correlation is 0.740, RMSE is 19.3 µg/m³, and bias is 0.8 µg/m³). This can be explained from the starting point of the processing (November 2018) beigin different from the main text (January 2019).

Additionally, in case (A) all months show negative biases, with the largest biases occurring in winter. This is likely due to the use of a fixed diurnal profile for residential emissions throughout the year (see Section S4). Introducing a seasonal component in this profile could improve the results.

2. The method used to estimate background NO_2 concentrations via a line integral over the municipal perimeter raises several questions:

a. Does $\mathbf{e_v}$ represent the local wind direction? If so, at what altitude or vertical level is the wind taken from?

We evaluate the wind direction at 10 m altitude at the centre of the domain. This wind is taken homogeneous across the entire domain. (Note that this is the same wind which is used in the dispersion modelling.) This clarification has been added in Section 2.2.1.

b. Eq. 1 resembles a mass conservation approach, but it lacks a temporal term—how is accumulation of pollutants within the domain accounted for?

Please note that the line integral is not based on a mass conservation approach. Instead, it represents a partial integration over the CAMS concentrations found along the domain perimeter, finding a representative (uniform) background concentration which flows into the model domain. The vector $\mathbf{e_v}$ is needed to (a) discriminate between concentrations flowing into the domain and out of the domain and (b) put more weight to line segments perpendicular to the wind direction.

c. Since the method depends on integrating along the perimeter, does this imply that the background concentration depends on the chosen perimeter?

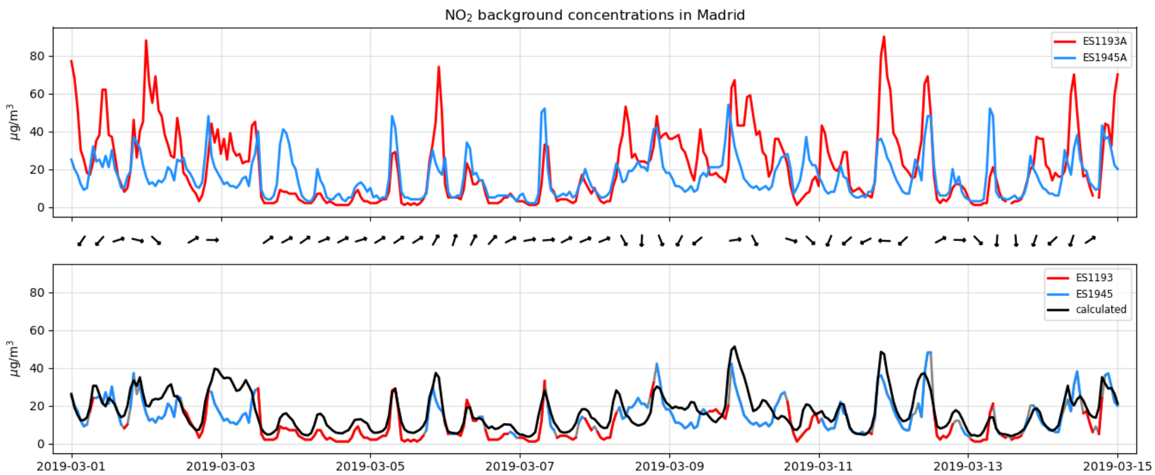
In our approach the background concentration is a scalar added to the locally produced NO_2 field. Changing the domain (or perimeter) will indeed alter the estimated background concentration. However, it also affects the calculated field of locally produced NO_2. As a result, the net effect remains relatively insensitive to the specific choice of domain boundary.

d. In the special case where $\mathbf{e_v} \cdot \mathbf{n}>0$ for the entire perimeter (i.e. all wind is outflow), the integral appears ill-posed. How is this handled in the analysis?

Since we assume a homogeneous wind across the entire domain rather than using local wind variations, this situation cannot occur.

e. Is this a novel approach? If so, could the authors justify its use and provide a comparison with background concentrations derived from station data within the domain?

To our knowledge, this is a novel approach. It is motivated by the need for a straightforward method to estimate background concentrations using the coarse-resolution data from the CAMS regional ensemble, while avoiding double counting of NO_2 from local emission sources. Validation of this method is now discussed in Section S1 of the Supplemental Material, based on the figure below.



The top panel shows NO_2 measurements from two suburban background stations: ES1193 (Casa de Campo) and ES1945 (El Pardo), which consistently record the lowest concentrations in the area. A third station, ES1946, also classified as suburban background, is excluded due to its elevated readings, likely influenced by nearby urbanization and proximity to Barajas International Airport. The time series show that the lowest NO_2 concentrations alternate between the two selected stations. This variation is partly explained by wind direction, represented by black arrows indicating 6-hour intervals. Typically, El Pardo registers lower NO_2 levels when clean air arrives from the northeast to northwest, whereas Casa de Campo, being downwind, includes additional local pollution contributions.

The bottom panel compares the lowest NO_2 concentration measured between the two stations with the background concentration calculated from CAMS data along the partial municipal perimeter, as described in Section 2.2.1. The close agreement between the calculated background and the observed minima suggests that this method provides a realistic estimate of background NO_2 under varying meteorological conditions.

3. The manuscript suggests that the added value of TROPOMI measurements becomes negligible when data from 5 or more stations are available. However, this rule of thumb may not be sufficiently robust, as it oversimplifies the issue. Other factors (such as city size, NO_2 concentration levels, local meteorological conditions, …) can significantly influence this threshold.

We agree that the rule of thumb regarding the added value of TROPOMI in relation to ground stations is not universally applicable to other cities. Accordingly, we have revised the corresponding paragraph in the Conclusion to present a more nuanced statement:

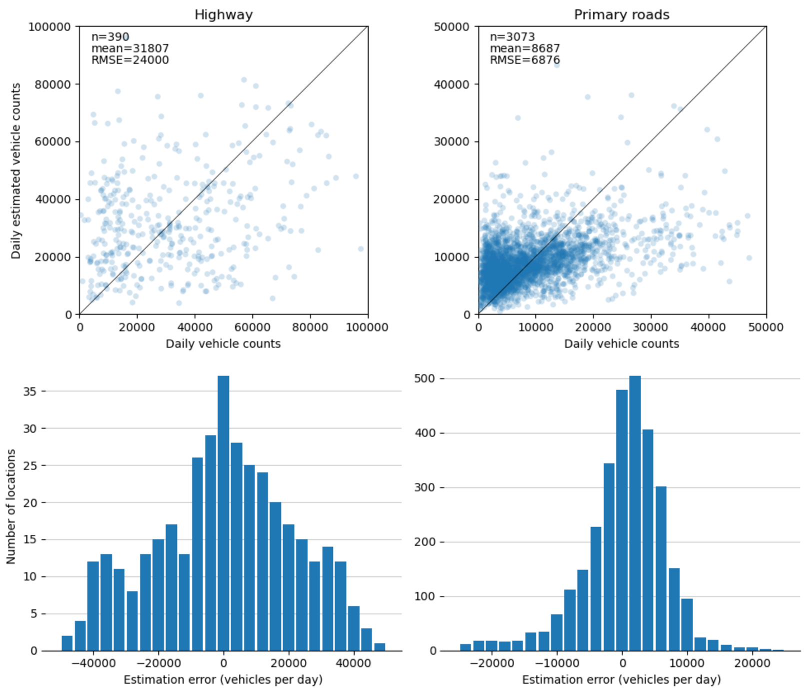
"The assimilation experiments for Madrid indicate that the added value of TROPOMI NO_2 measurements becomes negligible when hourly data from five or more ground-based stations at representative locations is available. *However, this rule of thumb cannot be directly applied to other cities, as the contribution of TROPOMI depends on various factors, including city size, NO_2 concentration levels, and local meteorological conditions*. Nevertheless, in many urban areas—especially those with sparse in situ monitoring—TROPOMI has the potential to provide substantial added value. Among approximately 2800 European cities with a population over 50,000, the European Environment Agency's AirBase (EEA, 2018) lists 2035 cities with at least one NO_2 monitoring station, but only 71 cities with five or more NO_2 stations (see Table S1)."

4. The manuscript states that traffic flow between counting locations is estimated using inverse-distance weighting interpolation, applied separately for highways and primary roads. However, since traffic volumes can vary significantly over short distances, especially in complex urban settings, this method might lead to unrealistic flow patterns. Could the authors justify the use of this interpolation approach and provide information on how its performance was assessed? Specifically, has any cross-validation been performed (e.g., removing some sensors and comparing interpolated vs. observed counts)?

Indeed, we recognize that traffic volumes can vary significantly over short distances in urban environments, and that inverse-distance weighting (IDW) interpolation may not fully capture such local variability. Our choice of this method was driven by the need for a practical and computationally efficient approach that could be applied consistently across many road segments, given the spatial resolution and availability of traffic data.

To assess the performance of the interpolation, we conducted a leave-one-out cross-validation based on daily traffic volumes. This was done separately for highways and primary roads, in line with how the interpolation algorithm is applied in Retina. For highway locations (n = 390), the average observed traffic volume was 79.5 vehicles per minute, while for primary roads (n = 3073), it was 6.2 vehicles per minute.

The resulting scatter plots of observed versus interpolated daily traffic volumes are provided below. Performance metrics are summarized in the table, reported as error ranges in vehicles per minute. The correlation is relatively low, supporting the reviewer's concern and highlighting the limitations of the current approach. We have now noted this explicitly in Section 4.1, where we emphasize that improved representation of traffic emissions—especially methods that better account for the relative distribution of traffic volumes—would be a valuable enhancement and are a priority for future development.



Error range (vehicles per minute)	Fraction of primary road locations within error range	Fraction of highway locations within error range
±1	23.1 %	8.5 %
±2	41.9 %	14.6 %
±3	57.3 %	19.7 %
±4	70.2 %	23.1 %
±5	79.1 %	26.2 %
±6	85.7 %	31.0 %
±7	90.3 %	37.4 %
±8	92.8 %	40.8 %
±9	94.1 %	44.4 %
±10	95.5 %	47.2 %
±11		51.8 %
±12		54.9 %
±13		57.4 %
±14		59.7 %
±15		62.8 %
±16		66.9 %
±17		69.0 %
±18		71.3 %
±19		72.3 %
±20		75.6 %

5. Pg. 27 line 518: The manuscript compares the Retina model's performance in Madrid with that of Kim et al. (2021), who trained a model using TROPOMI and 340 reference stations in Switzerland and northern Italy, obtaining a similar spatio-temporal correlation (0.79). However, several important differences limit the validity of this comparison: (i) Kim et al.'s study covers a much longer period (June 2018 to May 2020), including winter months, when satellite data is more frequently missing due to cloud cover—especially in complex alpine orography, which also affects the satellite's ability to translate column densities into surface concentrations. (ii) Elevated regions like the Alps can introduce systematic biases in satellite-derived NO_2 due to vertical gradients in NO_2 distribution and reduced sensitivity near the surface. (iii) Additionally, the amount of stations is much higher in the Kim et al. study (340 stations vs. 24 in Madrid), making their results spatially and statistically more robust. I suggest the authors reconsider the framing of the comparison or add more nuance to highlight the limitations and contextual differences that affect model performance in each case.

We agree, and now better frame the comparison between Retina and the mentioned machine learning approaches:

"Alternatively, several studies use a machine learning approach to generate hourly surface concentrations maps from a collection of data sets. *While our study focuses specifically on the urban area, these approaches typically cover larger regions and incorporate a broader and more diverse set of in-situ measurement locations.*"

Minor comments:

1. pg 9 line 199: "See 0"
2. pg 17 line 360 "Sect. 0."
3. pg 21 line 447: correct "Sect. 0"

All broken references have been restored.

4. pg 26, the manuscript states that "Direct assimilation of NO_2 satellite observations is not very useful due to the relatively short lifetime of NO_2 [...]" I would suggest that the issue may not lie in the inherent utility of the data, but rather in how the data is adapted and integrated into the model.

We clarified our motivation for using TROPOMI data to estimate emissions, rather than directly updating concentration fields, by revising this sentence to: "As a result, directly assimilating NO_2 satellite observations into concentration fields has limited utility, given the short atmospheric lifetime of NO_2 which limits the system's memory to just a few hours."