Review of "Optimal selection of satellite XCO₂ images over cities for urban CO₂ emission monitoring"

Alexandre Danjou¹, Grégoire Broquet¹, Andrew Schuh², François-Marie Bréon¹, and Thomas Lauvaux^{1,3}

¹Laboratoire des Sciences du Climat et de l'Environnement (LSCE), IPSL, CEA-CNRS-UVSQ, 91191 Gif sur Yvette, France ²Cooperative Institute for Research in the Atmosphere (CIRA), Colorado State University, Fort Collins, USA ³Molecular and Atmospheric Spectrometry Group (GSMA) – UMR 7331, University of Reims Champagne Ardenne, 51687 Reims, France

Correspondence: Alexandre Danjou (alexandre.danjou@lsce.ipsl.fr)

We would like to thank both reviewers and the editor for the careful and detailed reviews and their patience during this process.

It seems to us while reading the reviews that the aim of the study and of the different analysis conducted were not sufficiently explained, which perturbed the reviewers and undermined the comprehension of the links between the different parts. We thus

5 have made numerous changes on the introduction and took time to better introduce each sections. We have also changed the title as we found that it might give the impression that we used a model for our inversions, whereas we only use our model to generate our synthetic images. The description of the learning method has also been completely rewritten to make it clearer. Multiple comments were in relation to the article Danjou et al. 2024. This article is now published and accessible (https:

//doi.org/10.1016/j.rse.2023.113900). Some of the references to it were unecessary and have been removed. We also tried as much as possible to gather the references and explain them when necessary. We hope that the article is now more self sufficient

in regard to Danjou et al 2024.

1 Review 1

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In this manuscript, the authors discuss a methodology to estimate CO_2 emissions by cities in an automatic way to validate selfreported emissions by cities. For this, they use CO_2 concentrations simulated by a global model with an adaptive horizontal

- 15 resolution enabling them to increase the resolution to about 23 km² locally around 31 cities with improved representation of the meteorology and potentially better comparability to satellite measurements around these targets. Their methodology consists of calculating hourly XCO₂ during local daytime from their simulation in a 150x150 km² region around the city and then derive criteria to select images which they conclude will be appropriate for satellites to observe the emission plume using instruments like OCO-3 or CO2M. While it is an important scientific topic the authors try to tackle, the descriptions in the manuscript are
- 20 confusing and have many imprecisions making the manuscript hard to follow, which is why I suggest major revisions before the manuscript should be even thought of being published. In addition, it seems that the manuscript has been submitted in a

preliminary stage because almost no abbreviations have been defined, some values are "xx" (e.g., L496) and there are many typos in the figures. My comments are separated in general and specific comments, followed by technical corrections.

We'd like to thank the reviewer for his detailed comments. We apologize for the typos and other mistakes, which have been
left during submission. We acknowledge that these highlight a need for a better proofreading of our manuscript. We have now carefully reviewed it which has led to a significant improvement of the whole document.

1.1 General comments:

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- Citation Danjou et al. (2024): While it is appreciated that it is made clear by the year number 20xx that it is a preprint under review, the whole manuscript is based on this non-published study (cited 40 times). In order to make the results of this current manuscript understandable for the general public, it is important to add a comprehensive overview with all the results from your previous study needed to understand the results in this manuscript. In addition, please add the journal the manuscript has been submitted to so that at least it may be found in the future. You could also consider to publish the preprint in a citable space and cite this here, which would make this manuscript here much more transparent at this stage.
- 35 There may have been a problem in the process of sharing the files with the reviewers (we apologize for this failure). We actually sent the manuscript of Danjou et al. (2024) to the reviewers to support the review. As planned at that time, the paper Danjou et al. (2024) had been accepted in RSE and is now published.
 - It is never defined which is your reference determining the "error" which is mentioned at many points in the manuscript (e.g., L7, L91, L362 and many others). Unless the reference data of the city emission is not clear, the whole error analysis does not make sense, so please describe clearly what you use as a reference at some point of the manuscript. See also specific comment for L362. In addition, this also means that the motivation of this study is not clear: Are you investigating how well suited different methods are to determine emissions by cities (model as "true" emissions and method as uncertainty) or are you interested in which cities and meteorological conditions are best for analyzing city emissions with satellites, which is suggested by the title but where it is unclear what is your reference?
- The first proposition of the reviewer corresponds to the aim of the article Danjou et al. 2024. Here, as he precisely pointed out in the second proposition, we are interested in which cities and meteorological conditions are best for analyzing city emissions with satellites. We have replaced in the forth paragraph each occurrence of "this study" by "their study", when it was designating Danjou et al. 2024, as it must have been part of the confusion. We have also rewritten the 6th paragraph of the introduction and included a definition of the error : "As we are working with synthetic data, the error in the emissions estimate is directly accessible by comparing the emissions estimated by the inversion method with the synthetic true emissions used in the OLAM simulations."

The 6th paragraph is now : "The objective of our study is to resume the series of analysis from Wang et al. (2018); Schuh et al. (2021); Danjou et al. (2024) and deepen the evaluation of the conditions corresponding to reliable estimates of urban CO2 emissions using satellite XCO2 images. To do this, we use a little more than a month of simulations of

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- 55 local XCO2 scenes over large cities. This simulations are generated with the global OLAM model and evaluated by Schuh et al. (2021). We use these simulations to generate synthetic satellite images for the selected cities, and estimate their emissions by applying one of the automated and computationally-light inversion methods implemented, tested and optimized by Danjou et al. (2024). By using realistic simulations to derive the synthetic image and using a method independent of the model used for the simulations to estimate the emissions, we take into account realistically the uncertainty in the meteorology, atmospheric transport and background. As we are working with synthetic data, the error in the emissions estimate is directly accessible by comparing the emissions estimated by the inversion method with the synthetic true emissions used in the OLAM simulations. The study of the emission estimation error for different cities and weather conditions aim to support the identification of criteria for discriminating between images, separating those whose processing yields statistically reliable estimates from those whose processing is statistically unreliable."
- A major issue with satellite observations are clouds which will decrease the coverage. They are not mentioned in the methodology description (Sect. 4) in any way, but will probably be the main limitation to the emission estimates. I'm sure you can derive cloud information from your simulations which in my opinion has to be the first criterion to select whether emissions can be estimated using satellite measurements. This cloud screening would be something like a pre-selection of the images. Otherwise, the selection of the images is not "optimal" as suggested by the title.
- 70 When it comes to determining which cities are most suitable for measurement, cloud cover is indeed a major issue, and the frequency of cloud cover is an important criterion for city selection. We examined this point in section 6.2.

We have reserved this analysis for discussion because realistically adding the effect of clouds in images (filtered pixels and contamination of neighbouring pixels) and trying to objectively quantify their impact on error is of a complexity that would merit a dedicated study to do it more properly than what is proposed in the discussion.

We also believe that, once an image is partly contaminated by clouds, it is not worth processing. Indeed, the effect of cloud presence on the measurement is very complex, due to the presence of 3D cloud radiative effects in OCO-2 retrievals (https://doi.org/10.5194/amt-14-1475-2021). Given the size of these effects (of the order of a few kilometers) and the size of our images (a few tens of kilometers), we doubt the value of trying to obtain an estimate from an image contaminated by clouds. However, this remains to be demonstrated, and the complexity of such a task requires, in our opinion, a complete study and has no place here.

Adding clouds would not alter the conclusions we have reached, the criteria identified should still be important even in the presence of clouds. Thus, adding cloud coverage would only increase the error and add another criterion.

- It seems as if it is not accounted for detection limits of the satellites at any point in the manuscript and should be considered or at least mentioned somewhere. Can a satellite like OCO-3 or CO2M even distinguish emissions in the order of 2.1kt/h from the background?

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The term detection limit is often used in the context of the detection of unknown sources (methane super-emitters, for example, such as in Lauvaux et al, 2022). Here the problem is different: we already know the location of the sources (we

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know where the cities are) so we don't have to detect them but "just" to quantify their emissions. The term quantification limits is therefore more relevant. It is in fact the whole point of the article : to determine what conditions make it possible to quantify a city's emissions by satellite. We show that the city's emissions is one of the two most important criteria and we quantify a threshold on it and the error associated.

- All the results are based on simulations by the OLAM model, but the description of the model and of the performed simulations are not comprehensive, many things are missing making it hard to understand, see specific comments below for lines 95 to 138 and for Fig. 1.
- 95 See our answers to the cited specific comments. We have also took care to more broadly revise this section and hope it is more understandable now.
 - You are mentioning at various points in the manuscript that you are interpolating and extrapolating without including information which methods are used and why you are using them. Do these interpolations to a 1x1 km grid influence the simulated emission fluxes? Are they mass-conserving? Why and where are you extrapolating the XCO₂ values (L173)?
- 100 Common practice is to use the average of the background region. What is the reason that you use another procedure? Interpolation (l. 125 and 132) concerns the creation of images with 1km by 1km square pixels from data supplied by the OLAM model on a hexagonal grid. This interpolation is classic and conserves mass. It's all part of the synthetic-image generation process and not the inversion method.
- Concerning the extrapolation, Danjou et al. 2024 shows that using the mean to estimate the background is a very inaccurate estimator, hence the choice of a more complex extrapolation. We won't go into more detail here, as all this is described in detail in Danjou et al. 2024 (now available).

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- I am missing a description how you suggest to use your method for real measurements. How do you suggest to derive the variables needed for the analysis with your method with respect to real satellite measurements?
- Add to lign 295 : "When using real satellite images (which is out of scope of this study), meteorological variables can be derived from weather products such as ERA-5 (Hersbach et al., 2018). City characteristics can, as in this study, be calculated from gridded inventories sur as ODIAC, and from database on urban land cover and population/socioeconomic activities such as GRUMP."
- I would prefer reordering the methodology section because it is hard to follow in the current setup. First, I suggest putting the figure and table from Appendices A and B (Fig. A1 and Table B1) to their place in the main text where they are discussed as they have not any description in the appendices anyway. Second, it would be much better to move the descriptions from Sect. 5.2 to the decision criteria selection part in Sect. 4.2 and move the list of variables before this. This would improve the readability because otherwise, the reader is left with the methodology without the outcome in the current Sect. 4.2. We have moved the table in the article. Concerning the figure, we think that its interest is merely illustrative and that the space it would take up in the main body is far too large compared to its interest.

- 120 Concerning the reorganisation of the sections, most scientific articles present the method and the results in a separate way. Here we are following the usual order and think that mixing the two would destabilise the readers. We have also made it clear that parts 4.1 and 5.1 go hand in hand and form a preliminary analysis and rewrote the introduction of the sections to make the links and justification of the different sections clearer.
 - At some points you basically say that this is still work in progress and that your method is not applicable to all cities (L320, L324, L527) because it may depend on the surroundings of each individual city, which is okay but then the abstract should provide this information. We have added at the end of abstract : "Despite this efficient filtering, the accuracy of the estimates varies widely from city to city within the group identified as the most accurate."

1.2 Specific comments:

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- L1: define XCO₂ changed to "CO₂ column-average dry air mole fraction (XCO₂)".
- L4: "using synthetic satellite images": Please give more information how these images are generated in the abstract since this is part of this study. Addition of the abstract of : "It uses synthetic data experiments with synthetic truth and 9920 synthetic satellite images of XCO2 over 31 of the largest cities across the world generated with the global adaptive mesh Ocean Land Atmospheric Model (OLAM) zoomed at high resolution over these cities. We use a decision tree learning method applied to this ensemble of synthetic images to define criteria on these emission and atmospheric condition for the selection of satellite images."

L6: Success rate of what? Replace "has a success rate of 92%" by "manages to produce estimates for 92% of the images"

L7: Which cities did you choose? Please elaborate a bit. *replace "cities worldwide" by "of the largest cities across the world."* L8: What do you mean by "error"? What are you comparing with? *Error on the emission estimate. The answer to the following comments makes this comment obsolete.*

140 L8-10: The sentence starting with "Our learning method [...]" is clear: You already say that you reduce the error in the previous sentence. So I suggest to remove this sentence or rephrase. *Changed to "Our learning method identifies two criteria, the wind direction's spatial variability and the targeted city's emission budget, that discriminate images whose processing yield accurate emission estimates from those whose processing yield large errors."*

L12: Please define IQR Replaced "biais" by "median error" and "spread" by "InterQuartile Range".

L16: define UNFCC Replaced "UNFCC" by "United Nations Framework Convention on Climate Change (UNFCC)"
 L16: The citation has errors. Please consider putting the author in additional curved brackets. *citation corrected*.
 L25: define OCO The sentence has been rewritten and a definition of OCO has been added : "Observations of CO2 columnaverage dry air mole fraction (XCO2) at the scale of a few square kilometers from the two current Orbiting Carbon Observatory missions (OCO-2 and OCO-3) have paved the way for quantifying emissions from large (a few ktCO2/h) industrial (Chevallier)

150 *et al.*, 2022; Nassar *et al.*, 2017; Zheng *et al.*, 2019) and urban (Lei *et al.*, 2021; Reuter *et al.*, 2019; Wu *et al.*, 2018; Ye *et al.*, 2020) sources of CO2."

L28: please define ppm Add "-part per million-"

L30-33: Please add a citation for OCO-3 SAMs to this sentence. Add citep{Taylor2020}.

L38: define CO2M Definition added.

155 L38: define GOSAT-GW Definition added.

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L41: Please define WRF abbreviation. Add "Weather Research and Forecasting (WRF) model "

L46: "Attempt" could imply that these studies were not scientifically justified. Please rephrase. We have used this word to show that estimating emissions under such conditions bears large errors, as the quoted studies underline. However, to avoid any misunderstanding, we have followed the reviewers' instructions and changed "attempts to quantify" to "the quantification of".

L50: Sentinel 5-P does not measure CO₂. Please remove it. Indeed, sorry for this mistake.

L50: Please add a citation for GOSAT-2 reference to GOSAT-2 non pertinent and removed. "This is made possible by the launch of new satellites (e.g. OCO-2 and OCO-3) measuring XCO₂ at kilometer resolutions with ppm accuracy."

L51: define OLAM "Schuh et al. (2021) use high-resolution simulations from an adaptive-mesh model, the Ocean Land 165 Atmospheric Model (OLAM (??)),"

L53: I'm not sure what you mean by "variability of the local background signal". Within the surrounding of a small area like a city, the natural signal should be the same everywhere which is used for verification of the satellite instruments by small area approximation e.g. described by Taylor et al., AMT, (2023) and references therein. Please explain what you mean by that. *This statement is wrong : the natural signal shows high variability in the surrounding of the cities (see figure 1 for example). The*

170 typical variations of XCO₂ due to biogenic or anthropogenic emission and uptake, or even to changes in the wind conditions, are of a few or a few tens of kilometers, which is much finer than the size of our images. Thus the local background is variable within the image.

L57: Please remove "extensively" because this is a subjective rating. Ok.

L58: Please define in more detail what you mean by "pseudo-image". *Replaced "pseudo-images of XCO₂ concentration* 175 over Paris" by "simulated satellite images (i.e. synthetic images) of XCO₂ concentration generated with a meteorologicalatmospheric transport model over Paris". We replaced every occurrences of pseudo-images by synthetic images, much more accurate term.

L65: Please define IQR Definition added in abstract and l.65.

L76: I don't see any discussion of the uncertainty in the meteorology in this manuscript. Please explain. *The sentence was*indeed badly formulated and misleading. We wanted to express that, contrary to some studies we do not use the same model to generate the synthetic images and perform the inversion. We have rewritten this part : "By using realistic simulations to derive the synthetic image and using a method independent of the model used for the simulations to estimate the emissions, we take into account realistically the uncertainty in the meteorology, atmospheric transport and background."

L80-81: Please elaborate which configurations in the framework of Paris you are talking about. It seems to me that you do not rely on the same values. Please clarify and refine your definition of configurations here. *We have rewritten this paragraph* (*see previous comment*) and move this discussion to the section 3.

L87: Do you mean "evaluate" or "judge"? "indicate" is indeed more suited. We have replaced "we hope to indicate" by "this analysis is expected to support the development of tools to evaluate".

L88-89: If you want to mention the subsections here you should mention all subsections (Section 2.1 is missing). But I
would prefer introducing the subsections at the very start of Section 2. We have followed the reviewer suggestions and moved all the description of the subsections at the beginning of the corresponding section.

L90: The configurations are not "recalled" in Sect. 3. There's just always a reference to the non-published paper. So, please provide a comprehensive summary of your study somewhere in this paper, summarizing all results needed to understand it. *Replace "The inversion methods are described in Danjou et al. 2024 in their optimal configurations and are recalled in Section*

195 *3" by "Section 3 describes the inversion method used to make the emission estimations for the main set of analysis in this study. The results with the three other automated methods described in Danjou et al. (2024) lead to similar conclusions and their analysis is thus summarized in Appendix B."*

L91: Which "discrimination" do you mean? Please clarify. *We have rewritten the introduction and the term is now introduce earlier.*

- 200 L99-105: It is not clear to me from this description how the model exactly is setup: My understanding from this is that the grid box sizes in this model are flexible and can be adapted for a region of interest, while being fully coupled to their neighbours. On the other hand, it seems as if the parameterizations are also adapted for each grid box and I'm wondering how the authors can ensure mass conservation and general consistency in this model, e.g. at which grid size do you decide to switch from hydrostatic to non-hydrostatic mode? And is the time step the same everywhere in the model, and if yes, how do you deal with
- 205 the fact of wind speeds leading to motion across more than one grid box, especially in the higher resolution? A bit more details would be beneficial here. *The model is an icosahedral model, originally working in either the triangular or hexagonal dual spaces, but most recently being coded to mostly work in hex space. The mesh refinement procedure is documented in Walko2011 , and is also common place in other more well known icosahedral models such as MPAS (out of NCAR/US). Parameterizations working across spatial scales are obviously tricky and a constant research target. Currently OLAM uses a blend of the original*
- 210 Grell deep convection scheme with aspects of the Grell-Freitas scale aware scheme to accommodate this. Ref below explains mesh refinement procedure.

Walko and Avissar, A Direct Method for Constructing Refined Regions in Unstructured Conforming Triangular–Hexagonal Computational Grids: Application to OLAM, 01 Dec 2011, https://doi.org/10.1175/MWR-D-11-00021.1,3923âĂŞ3937

L96-105: In addition, you describe below that you simulate more than one month with the model. How do you achieve realistic meteorology in your model? Is it nudged towards an external dataset? Is it free-running? *It is initialized to realistic 3D met fields initially and then free running, i.e. forecast. In this sense, we get better internal consistency of tracer fields w/o the demanded jumps and so forth that would be required if you were forcing mass related variables, such as humidity and density, to external reanalysis. This is an area of active research now though since we'd like to use this model towards working with real observations at high resolution.*

around L106: What is the top altitude of your model? Does it account for troposphere, stratosphere or only the boundary layer? As satellites measure the total column XCO_2 this is an important information to be added. In addition, how many model levels does your model have and how well-represented is the lower atmosphere in the vertical, i.e. how many model levels are in the boundary layer and what is the vertical grid spacing there? *The top altitude is 37,503 MASL. The model is a full general circulation model (GCM), as described in Walko et al 2008a and Walko et al 2008b. In other words, yes, it handles all of that.*

- 225 The model edges are given below (in MASL, plus 0 MASL):
 [1] 50.0000 101.4817 157.6048 218.2211 283.6903 354.4010
 [7] 430.7727 513.2588 602.3487 698.5710 802.4969 914.7432
 [13] 1035.9758 1166.9143 1308.3357 1461.0792 1626.0514 1804.2312
 [19] 1996.6760 2206.3650 2438.7712 2695.6487 2979.5740 3293.3953
 230 [25] 3640.2603 4023.6484 4447.4058 4915.7822 5433.4766 6005.6816
 [31] 6638.1367 7337.1865 8109.8428 8963.8555 9907.7920 10951.1201
 - [37] 12104.3057 13378.9160 14787.7373 16344.8994 18066.0234 19968.3730
 - [43] 22045.2324 24258.5957 26626.7012 29160.3691 31871.1738 34698.8203
 - [49] 37502.7891

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235 These are generated as 49 levels with fairly constant stretch ratios between levels to ensure optimal numerics.

We have added 1.106 " The model has 49 vertical levels (from 0masl to 37kmasl), twelve of them being in the first kilometre, which supports reliable simulations in the lower layers of the atmosphere, where the plumes are located."

L106-108: This is not correct. There are models that use altitude and surface following coordinates successfully. So please delete this sentence or at least rephrase. *Our statement was maybe a bit strong, and we have moderate it by replacing "is*

240 optimal to avoid" by "helps avoiding". However we have to say that we do not agree with the reviewer comment. Every kind of model (and vertical coordinates systems) have their advantages and disadvantages. This is a strength of OLAM and the used coordinate system. If the reviewer does still not agree with our statement, we can delete this particular sentence as it is not essential to the paper.

L108-109: I would prefer either to delete these general sentences about the model or move them above to the introduction
or the general description of OLAM above in this subsection. Otherwise, it is confusing with respect to the actual setup of the model in your study. *We moved upward (l.100) those sentences as suggested and mixed then in the first paragraph on OLAM.*

L109: What do you mean by "It [...] allows to reduce the representation of urban plumes"? Do you mean that you can simulate the plumes more accurately using your approach? This sentence is indeed unprecise and we have rephrased it : "In our case, it allows us to realistically represent the urban plumes of a large number of cities and the underlying large-scale variations in CO_2 , while maintaining a global domain and an affordable computation time."

L110: Comparing the mentioned mesh size of 3 km with Figure 1 and the statements at the beginning of Sect. 2.3, it seems as if there is one value per hexagon, meaning that the grid points represent the hexagons with a side length of 3 km (according to Sect. 2.3) which does not mean that the mesh size is in this order. A more readable quantity would maybe an effective side length of a rectangle with the same area as the hexagon. *We agree that this metric is misleading. We choose the area of the*

255 *hexagon as more readable quantity, as suggested below.*

Sentence in L107-108: Does that mean that you use higher resolution at all coastlines and mountains on the globe in your configuration? Please clarify. *No, not necessarily. Dynamicists using a model like OLAM would apply mesh refinements in*

areas where dynamics, e.g. winds/pressure, would be expected to change quickly, e.g. mountain circulations, sea breezes, etc. This is the MAIN use of modeling constructs like this (in general). For us, we are conditioned on looking at cities so we're

260 interested in it for two things, (1) representation of high res emissions EVEN if the underlying meteorology doesn't change a lot across distance and (2) representation of high res emissions when the meteorology does change, such as cities near topography, e.g. Los Angeles, Lima, Bogota, etc. We have rewritten this sentences and hope that the changes resolve this comment.

L115: define ODIAC abbreviation *Replace "ODIAC" by "Open-Data Inventory for Anthropogenic Carbon dioxide (ODIAC)"* L120: Which method is used to interpolate the results to the regular grid and which target resolution is used? Does the interpolation have an influence on the results? *Add on l.121 "The XCO2 fields are calculated by the model on the hexahedral* grid. [The results of these simulations are then projected onto a regular grid] at approximately 1km×1km resolution. [This is done] to simplify the analysis of the model outputs."

Figure 1: Where do the large XCO_2 values in the very south of the left panel come from? When looking at broader image on the same day, it seems to be a plume coming from the city at the edge of the image.

Figure 1: It would be helpful if you could include an example where the pseudo-images are located in this figure. In addition, "twice the size" is wrong because it relates to the square edges in both dimensions, therefore it should be "four times". *Ok, location of the pseudo-image added. "twice" replaced by "three times", as the plotted image is a square of approximately 240km rather than 300km (changes made in the legend).*

L122: It seems from Fig. 1 that the mentioned regular grid is highly oversampling the native grid, but this should be noted
somewhere here. In addition, it is not clear from the description whether XCO₂ is calculated on the native grid and then interpolated or vice versa. *The regular grid is at 1km and interpolating 9km² sized hex grids, so somewhat oversampling. XCO2 is (and should always be) calculated on the native grid and then interpolated with these types of models (because of complexities w/ the unique irregular grid structure.) We added 1.120 "The XCO₂ fields are calculated by the model on the haxahedral grid. The results of these simulations are then projected onto a regular grid at approximately 1km × 1km
resolution."*

Figure 1 suggests calculation on the native grid and then interpolation, but the text describes it the other way. Please clarify. *We clarified this, see answer to previous comment.*

L125: The resolution should be moved upwards, including information how the data are interpolated. See comment above at L120. Done : answer to comment l.120 and changed "The original XCO2 fields on a variable resolution grid were interpolated
to a regular grid at approximately 1km×1km resolution, which" to "The model output resolution of 1km×1km"

L128: As mentioned above, if there's one value per hexagon, the area of the hexagon is most relevant here, which is 23.4 km^2 for the model, 3.1 km^2 for OCO-3 SAMs and 6 km^2 for CO2M. Therefore, the hexagons at the highest resolution are still 4 to 7 times larger than the satellite footprints. *There has been a misunderstanding on the size of the hexagons, which enforce the point of the reviewer on the need of a more readable quantity... The smallest cells have an approximate area of*

290 $9km^2$. Sentence changed to : "This resolution is finer than the finest resolution of the model's adaptive native hexagonal grid (hexagons of $\approx 9km^2$). Therefore, the variations of the model variables (XCO₂ field, wind field,...) have a spatial resolution which is coarser than the $1km \times 1km$ resolution of the model output grid, on which the analysis will be conducted." L129-130: "[...] on which the analysis will be conducted" What is the mentioned spatial grid? Is it the actual satellite footprints? *No. It is the 1km x 1km grid. Change integrated in the answer to the previous comment.*

295 L129: It is not clear which "simulated patterns" you are talking about here. Please clarify. *replace "pattern" by " variations of the model variables (XCO₂ field, wind field,...)", see previous comment.*

L130: Please provide the date notation in the standard format defined by Copernicus. In addition, these are 41 days, but obviously only 40 days are used to get the 9920 images. Please clarify. *The last day is excluded (simulation stops at 0a.m. on the 10th of September)*. It was effectively not clear. Dates changed to "08 August 2015 - 09 September 2015 (included)".

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L132: Please clarify where the number of 9920 images comes from, because 8 hours per day x 41 days x 31 cities does not arrive at this number. *see previous comment*.

L135: "that expected for CO2M" - Please mention the swath width of CO2M somewhere in the paper (maybe best in the introduction). addition in the introduction of the resolution and swath width of CO2M. Removal 1.127 of the parenthesis mentioning Sierk and the resolution of CO2M.

- 305 Section 2.3: I understand from your description that you interpolate your simulation results to a 1x1 km grid and use this as a proxy for what the satellite sees. It would be much better if you used real orbit data from both satellites and account for the actual footprints of them (which you do anyway in your preprint Danjou et al., 20xx). *The aim of this study is more general than just the OCO and CO2M data. Analysis with real orbits would not fundamentally change the results, as the main discrimination criteria should remain the same. An interesting point would have been to study the influence of image size and*
- 310 resolution, which are certainly important discrimination criteria, but this would require a separate analysis due to the number of images required.

L144-157: This procedure seems very complicated to me and also for the application to real satellite measurements. It would be great to have an illustration of the distribution of emission targets in a city and what is the benefit with respect to a simple circle of a specific size around the city center. I am sure there are reasons for you to do this procedure but it is not clear to

- 315 me what these reasons are from the description in the text. We have completely rewritten the introduction of this subsection to introduce the motivations more clearly : "The first task for urban emission estimation is to define the targeted emission zone. As the aim of our quantification is ultimately to help monitor actual emission reductions, we focus on the urban area corresponding to the most significant emissions rather than the actual administrative boundaries of the city. Consequently, the definition of the targeted emission zone is made regarding the size of plumes that can be detected in a SAM and by identifying
- 320 the most emitting pixels from the spatialized inventories (using a similar concept but a different and more straightforward approach compared to ?). Because the typical size of a SAM is about 80km × 80km, we set the size of the targeted emission zone at roughly the size of a 20km radius disc. Thus, the emission zone we target occupies around 20% of a typical SAM and 6% of our synthetic images. "

L164: If the metropolitan areas from GRUMP are larger than a SAM what is your argument to decrease their size in your study? If the only reason is that you decrease it so you can study it, this would be a recursive argumentation and not scientific. we indeed define a target size that we can measure. We don't see what the reviewer means by "recursive" and why our rationale is not scientific. Defining cities boundaries is not a simple task, as the political definition rarely match the economic or emitting zones. What are we interested in : the emissions of the political entity or of the economic zone? Keeping in mind that the target is to monitor emissions in order to help decrease them, we think that the emission zone is more important. The GRUMP database

330 choose a definition "based on a combination of population counts (persons), settlement points, and the presence of Nighttime Lights" (https://doi.org/10.7927/H4GH9FVG). We, given the fact, that we are interested in the emissions budget, are defining the city limits based on the a priori core of the emissions.

L165: I am sure you can redefine these metropolitan areas in the model to your definition (why should it not be possible?). By that, this analysis would become feasible and possible. *The simulations used in this study were not performed for this but for the work done at CSU, and for example the cited article Schuh et al. 2021. We are only users of them and don't have control*

over them. Doing this kind of simulations is very time-consuming and was not worth it for this study.

335

Furthermore, a second problem arises with month-long simulations with global models for defining the exact limits of a plume. For simulations with a restricted domain, the plume leaves the simulation zone at one point and does not return, which means that the tracer only keeps track of emissions that took place in the previous hours, and not the previous days. With a

340 global model, this "finite memory" of the tracer does not exist and the emissions from the days preceding the synthetic image, which should be considered as background, are still in the tracer, which makes exact identification of the plume impossible. As this paragraph perturb the reviewers and is merely a digression on the simulations, we have removed it.

Sect. 3: Instead of always mentioning the non-published manuscript and comparing with it, it would be much better to describe your methodology here completely, so that the reader canfollow your steps (or as mentioned in the general comments

- 345 provide a comprehensive summary of the other study at some point and refer to that). We have rewritten the first paragraph of this section : "The complete description of the inversion method and the details and justifications for its specific configuration and implementation can be found in Danjou et al. (2024). We make the assumption that the configurations chosen in the framework of their study remain optimal for other cities. This assumption seems justified, as the chosen methods for each steps differ from the discarded methods on objective criteria. This section only gives an overview of the different steps and
- 350 the adaptations (compared to the reference configuration from Danjou et al. (2024)) that were made in the context of this study." We also tried throughout the section to suppress the unnecessary citations of Danjou et al. 2024 and regroup as much as possible the necessary ones. We hope that it is now acceptable

L170: Also here, an illustration would be helpful. For instance, does this plume boundary account for the fact that the emission zone is an extended zone or does it just start in the center of the image? *This plume boundary account for the fact*

355 that the emission zone is an extended zone, as it includes "the pixels located above the city" (l.170). Illustration can be found in Danjou et al. 2024. We would rather not expand the description of the inversion method as its description is not the point of this article. We make it clearer on the introduction of the section that the inversion method comes from this previous study and hope that readers that are further interested in the method will look at this previous article.

L171: "over the entire image": For point sources such as power plants, only the wind at the location of the emitting target is usually used to determine the direction of the plume (e.g. Nassar et al., 2022). Although this is not a point source, I think the average should be taken for the emission zone, only. *Here we are interested in the direction of the plume over the city and it's neighbourhood. Indeed, we could have choosen a smaller zone to estimate the direction of the wind. However, this direction* is just a rough estimation that will be refined during the derivation of the centerline and during optimisation of the gaussian plume (as it is one of the free parameters). Therefore, we do not think that this point will make a difference in this study, but we

365 *keep it in mind for future work.*

L175: I think you mean an estimate of the enhancement in the plume. Indeed. Change "plume" by "plume enhancement"

L176: Is the 5 degree polynomial used because of changes in the wind direction? Can you estimate the emission when the wind is so variable? There will be also mixing into the plume when the wind varies in its direction which is why usually only times are used where the wind can be assumed to be uniform. *Yes. Cases where the variability is to high will be filtered*

- 370 according to the results of section 4. It has been already demonstrated that for wind slightly variable, we manage to have a more precise estimation with a 5 degree polynomial rather that just a line (Danjou et al. 2024 et Kuhlman2019). Discussing the inversion method is not the point of this article and thus we didn't detailed further those point in the section. However, we have put more emphasis at the beginning of the section that the method has been evaluated in a previous article and that the justification of the configuration should be found there. We hope that it is sufficient.
- 375 L182: "averaged wind" By that you already assume that the wind is uniform all over the analysis area and the PBL. Therefore, I do not understand the 5-degree polynomial mentioned earlier. The reason why we use average instead of value at the source is actually to account for the variability. Our inversion method require the use of a single wind speed value for the Gaussian model. The Gaussian model assumes an uniform wind, but we limit the impact of such an approximate assumption by feeding it with wind speed average over the right area.
- 380 The difference between using a 5-degree polynomial centerline or a linear centerline is quite small when looking at the error of the emission estimation, especially for the inversion method used here. But Danjou et al. 2024 et Kuhlmann 2019 found that it nonetheless gave better results, especially for cross-sectionnal inversion method and more complex gaussian model.

L186: Is W the horizontal wind? It's the effective wind, i.e. a 2D vector that simulate the average horizontal wind speed driving the plume. We have moved its definition to the l.182.

385 L187: The value in brackets of sigma should be x. Yes.

395

L187: "the mass of CO_2 in the atm. column per unit area" I assume you mean the enhancement in the plume? *change to* " CO_2 mass enhancement of the plume in the atm. column per unit area".

L190: It is very confusing to talk about "modelled" here, because it could also mean some XCO_2 modelled by your OLAM simulations. Please rephrase and mention that it's the Gaussian plume model you're using here. We think that the precision

390 of $\Delta\Omega_{gp}$ makes it quite clear what we are talking about. We nonetheless changed "between the modelled mass per unit area $(\Delta\Omega_{gp})$ and the observed mass per unit area. The observed mass" to "between the mass per unit area simulated by the Gaussian model $(\Delta\Omega_{qp})$ and the pseudo-observed mass per unit area. The pseudo-observed mass"

L191: Similarly to the previous comment: "Observed" is very confusing because you're using simulated values everywhere. Please rephrase. *We are very clear that we only use synthetic data in all this article. We do not see why the reviewer is confused. We nonetheless added quotation marks around the "observed".*

L192: Delta XCO_2 in the equation should be dependent on x and y. (x, y) added.

L192: As this equation seems to be a numerical value equation units should be given to the quantities. What is Delta XCO₂ here exactly? And I assume the M's are molar masses? $^{"}\Delta\Omega(x,y) = \frac{M_{CO_2}}{M_{dryair}} * \Delta XCO_{2obs}(x,y) * 10^{-6} * \frac{P_{s,dryair}(x,y)}{g}$, where g is the Earth's gravity (in m/s²), $P_{s,dryair}$ is the dry air surface pressure (in Pa), M_{dryair} and M_{CO_2} the molar mass of dry air (28.97g.mol⁻¹) and CO_2 (44.01g.mol⁻¹) and ΔXCO_{2obs} the observed plume enhancement (in ppm)."

L193: I would call the surface pressure $P_{s,dryair}(x,y)$ because it depends on the x and y direction. Done

400

L194: The description would be much clearer if you would mention that r, a and F are free parameters in Eq. 1 which you want to fit here to get the best estimate in terms of the Gaussian plume model. *"are optimized during this minimization." replaced by "are free parameters in equation ?? that are optimized during this minimization."*

405 L197: Where does the "average" radius of the city come from? Addition "[noted r^{init}]) defined as the square root of the city surface divided by π ."

L201: Why is the normalisation needed? And why are you using exactly this normalisation? Please add this information here. *Despite not being necessary, it is usual to rescale data during optimization to facilitate convergence.*

L202: "for clarity": Why did you choose these limits? Please explain. Addition l.203 of "This bounds are fixed to avoid 410 unrealistic results (e.g. detected plume direction perpendicular to the wind, high CO_2 uptake from the city,...)"

L203: The angle should be "Theta" and not "Theta_init" and the "Element" symbol is missing. Indeed : $\theta^{init}[\theta^{init} - \pi/4; \theta^{init} + \pi/4]$ is changed to " $\theta \in [\theta^{init} - \pi/4; \theta^{init} + \pi/4]$ ".

L204: "defined as optimal by Danjou et al. (2024)". Please provide a summary of the non- published manuscript somewhere in the paper with all the results needed to understand this study. *Following the numerous remarks of the reviewer of the citation*

- 415 of Danjou et al., we scan this article for every occurrences of this citation and removed those who were unnecessary. We also tried to regroup them on a just a few necessary places and improve the references. For this particular place we think that it is necessary and the removal of numerous references above makes it less annoying. around L210: The description would be much clearer if you would mention that the actual shape of Paris is nearly circular
- whereas this is not generally the case for all cities, which is why you had to adjust the radius of interest. We removed all the
 parts concerning adaptation of the plume boundary definition. Indeed, it was not the plume boundary definition that changed compared to Danjou et al. 2024 but the city definition. The changes described were only the impacts of the new definition of the city boundaries, and thus not relevant.

L211: What does "4.3" mean? Please clarify. It is the section of the Danjou et al. in which the info can be found. Sentence has been removed following answer to previous comment.

425 L215: I do not understand what you mean by "directly above the city". From my understanding, you have to estimate the emission downwind of the emission target. Please clarify. *Those are the pixels above the city. We removed this part as it was not relevant, and may partly explain the reviewers incomprehension.*

L218: As the IME abbreviation is not in the main text, it would be better if you defined it in the Appendix C where it is actually used. *parenthesis removed and addition of IME 1.540 (section C1)*

430 L221: appendix -> Appendix C (or actually Appendix A if the Appendices A and B are removed as suggested above) *see choice made in previous comments*

L222: I think you would like to do an error reduction of your analysis, so please rephrase the title accordingly We do not understand what the reviewer meant by this comment. However, we agree that the title needs to be expanded for clarification. Title changed to "Analysis of the sensitivities of the emission estimation error to observation conditions : general principles"

435

L222: Please explain first what you mean by the "sensitvities" and what is the general purpose of this section before going into the details. Addition at the section beginning of "To identify the main criteria of classification of the images based on the performances of the emission estimation, we analyze the sensitivity of the emission estimation error to the different variables characterising the observation conditions and the inversion. We thus can see which variables are influencing the most the emission estimation error, and define criteria, based on those variables, determining whether a pseudo-image is suitable for emission estimation or not."

440

L229: You have not mentioned how the error on the emission estimate is calculated before. Please add this information to the previous section about the methodology. A definition is now present in the introduction.

L231: As mentioned above, it is not clear from your description why you are doing this sensitivity analysis. A motivation for this is needed. A paragraph has been added at the beginning of the section to describe its motivation.

445

L233-234: "a way to define ...": This is the motivation. Please move this to the front of the section. See addition at the beginning of the paragraph (answer to comment about 1.127)

Sect. 4.1: I think you're saving here that you are binning your images according to percentile thresholds in 5% steps. But it is not clear from your description if you do this for each city separately. We do not do this for each city separately, as you can see by the number of images in each bin.

450 L263: "variance reduction": So your error mentioned earlier is the "variance"? Please explain. No. This is a general description of a decision tree algorithm functionment. Here, we have removed variance reduction and instead use the term "loss *function*" *for clarity*

L266: "the depth is set to 2": You do not mention here, which criteria are used in the end, which is confusing. It would be better to combine this discussion with Sections 5.2.1 and 5.2.2 where the criteria are discussed, also because the second

choice ("diagnostic" variables) depends on the first choice. The criteria selected by the tree are the main result of our analysis. 455 We would rather keep the separation between the method and result section and describe the found criteria in section 5. The description of the decision tree as be rewritten and we hope that it is clearer now.

Sect. 4.2.2: It seems as if your decision tree is a two-step procedure: First, you do it for the predictable variables, then you do it for the remaining images using the diagnostic variables. Please include this information somewhere. Indeed it was not

- clear and was undermining the comprehension of this article. We hope that the developments of the introduction of section 4 460 answers this comment (particularly the addition of "The two types of variables are analysed separately as they can answer to two different questions. The predictable variables can be used before the inversion to determine if an image will give a reliable emission estimate and is thus worth acquiring and inverting. The diagnostic variables are accessible only after the acquirement of the image and the inversion, and can thus just give an indication on the reliability of the emission estimate.".
- 465 L285-286: The sum of the number of variables in brackets do not match the ten diagnostic variables. "8" replaced by "9" in the brackets.

L286: I think it would be appropriate to put the table here as part of the main text. Otherwise, the reader has to go to the end of the paper to understand what you are referring to here. *Ok*.

L290: There are many peer-reviewed publications highlighting the importance of wind in the calculation of emissions from 470 emission targets, so please use another publication here. *The sentence does not say that "the wind is important in the calculation*

of emissions from emission target", but that there is a correlation between the accuracy of the emission estimation and the mean wind speed or the wind spatial variability, which is a more precise statement. We have added a reference to Feng2016.

L294-298: So your suggestion is to apply exactly this method with the same thresholds to real satellite data for these cities? *Yes.*

- 475 L299: You have already characterised the background XCO_2 in the sections before. Do you mean you want to characterise the variability of the background because this could lead to errors? *Change l.* 299 and 300 by "To characterise the complexity of the background XCO_2 field in the image, we use the spatial variability of the XCO_2 concentration. This variable has been highlighted by Danjou et al. 2024 as being correlated to the error on the emission estimation. Indeed, a high variability of the background leads to an estimation of the background concentration (step (iii) of the inversion method) less accurate and thus
- 480 an error in the plume enhancement estimation, and thus in the emission estimation." We hope that it clarifies the difference between this "backround variability" and the background estimation defined earlier.

L300: It is clear that the background is crucial for the analysis of the emission plume. There are many publications highlighting this, so please use another citation for this. *We are not talking about the importance of getting a precise background estimation, but of the fact that the error on the emission estimation is correlated to the variability of the background inside*

485 an image. We have developped the description to make our point clearer. To our knowledge, not many studies pointed out this relation as clearly. We hope that the changes made following the previous comment helped clarify our point.

L303-304: It is your choice to define a fixed size of the images. You could easily include a variability in the size of your images to analyse this effect, e.g. by adding a random parameter to the edge size of the images. Because you're saying this could be important this would be worth doing. *Indeed this would be interesting and we keep this in mind for further study. But*

490 we think that the number and type of variables studied are already important and adding one won't affect the importance of those we highlighted.

L314: This is the very first mentioning of GP2. Please define what you mean by that. Typo. Replaced by "our".

L314: It is unclear from the description where this number of 92% comes from. Please extend your explanation. Addition of ": in 8% of the cases, the optimisation does not converge"

495 L315-316: Does that mean that the uncertainty of your method is 78% which would be huge and mean that we basically cannot infer much information from that? Please clarify. An illustration of this would be helpful, too. *Indeed the uncertainty is huge. Rather than saying that we cannot infer information, we would say that to infer reliable information we need a lot of images, as the method has nevertheless a small bias. Figure 3 and 5 give illustrations of the bias and spread of the method. We added l. 316 : "Reducing the bias and spread of this distribution is essential in order to obtain usable emissions estimates."*

500 L320: "the variability of the error distribution remains large across cities": Again, an illustration would be very helpful here to understand what is meant by error distribution. *The error distribution is now explained earlier, following previous comments, which should make it easier to grasp what those percentages mean.*

L324: Are you saying here that your method can only applied to single cities? *We don't understand the reviewer comment. Our method can apply to every cities in the world, but the bias and spread of the emission estimation distribution will depend of the city characteristics and the meteorological conditions. We have modified the sentence and hope its meaning is clearer now*

: "The strong disparity of the error distributions between cities suggests that the error on the emission estimation is sensitive to the city characteristics (topography or city-specific atmospheric conditions) and/or to the city emissions (spatial distribution, magnitude,..)."

L331: "significant": Did you check for statistical significance here? If not, please replace by "increased". *Replaced " are impacted by significant errors" by "show an important bias (see Fig. 3)."*

Fig. 3 caption last line: left-hand -> right-hand Done.

505

525

L335: Since Appendix C has many subsections, please refer to the correct subsection here. Reference changed to C.2.

L337: "impairing our ability to determine the optimal set of thresholds": If the variables are correlated they do not provide additional information, so you should choose independent variables. *The point of the study is to determine which variables*

- 515 are the most important between those correlated variables. We are looking for the ones that provide the most information. As we are unable to determine them using the preliminary analysis, we have decided to use a decision tree learning method. The last paragraph is replaced by "The error in estimating emissions therefore shows sensitivities, sometimes complex, to several variables, some being related, again in complex ways. Because of those intricated sensitivities, the simple analysis conducted in this subsection is insufficient to determine the optimal set of variables and thresholds for defining the most optimal
- 520 discrimination criteria for the synthetic images. This justifies the use of a more complex learning method. The supervised learning method described in Section 4.2 will enable us to determine the discrimination criteria more objectively, despite the covariances among the variables."

Section 5.2: These results should be moved to a much earlier place, because otherwise the manuscript is hard to follow. See our previous comments concerning the suggested reordering of the sections. We have developed the introduction of each sections and hope that it make our study easier to follow.

L352-357: I think what you want to say here is that you calculate the median threshold and remove all data that are beyond the threshold where the error increases. Please clarify. *Not at this stage of the study, we do not yet focus on "data that are beyond the threshold where the error increases". We made some changes to clarify. l.355 "The emission budget distribution" is changed to " The distribution of the threshold on the emission budget". "The distribution of the criteria is" changed to "The*

⁵³⁰ distribution of the thresholds are". 1.357 Addition of "For a given pair of criteria among the 82 retained, the subset giving the lowest error is that formed by images whose spatial variability of wind direction is below the threshold given by the decision tree and whose emission budget is above the threshold given by the decision tree. [The 82 subsets are] " 1.357 Removal of ", however,"

L354-355 and L356-357: Why is it important how many images are between the bounds? I do not see the importance of these sentences. *To see the stability of the criteria*.

Fig. 5 caption: It would be good to add the absolute emissions of the 31 cities you investigated at some point of the manuscript. Do they differ by many orders of magnitude? *addition of the emission budget on a twin x axis of figure 5*.

Fig. 5: From the description in the main text, I think the values on the y-axis are not given in percent but in ratios to the emission. *yes indeed. The label has been changed. "GP2" replaced by "gaussian plume" in legend.*

540 L362: Since it is not explained at all in this study up to now, where the "error" comes from, this statement cannot be validated. Please explain in detail at some point how you define and calculate the error in your analysis. *Addition of "in their framework (perfectly known background concentration, simplistic simulations of the urban plumes)"*. A definition on what we call the error on the emission estimation as also been added following previous comments.

L424: Please repeat these here or somewhere else in the paper since your previous study has not been published yet. *The study has now been published in Remote Sensing of Environment.*

Fig. 6: Please add numbering to the panels and refer to them in the text. Otherwise, it is not clear which panel you are referring to. *Ok*.

L448: The orbit of OCO-3 is not really predictable so that the overpass can happen at any local time during daytime. Please clarify. "These different times are chosen to be representative of the times when OCO-3 passes through." replaced by "These different times are chosen to sample possible times of OCO-3 overpasses".

L449: Why are you using 11° here and not 12°? This is an error, 12 is the right number.

550

L451: It is clear that a lower resolution will result in smoothed and more homogeneous wind speeds/directions. Addition of "and thus leads to smaller values of the spatial variability of wind direction".

L452: As mentioned above, the resolution of your model is not 3 km but rather something around 5 km. *This was a miscomprehension due to a very poor description of the model from our side. This has now been changed.*

L453: "are located in Asia and America": Which is surprising because these cities have supposedly the highest emissions. How do you explain this? *As we say in the mentioned sentence, we are just looking at the criterion on the spatial variability of the wind direction, in this case.*

L456-460: This should be mentioned much earlier. Please mention at your earliest convenience that you are interested in 560 clear-sky conditions only here. *Addition in the description of the synthetic images of "We do not take clouds into account when generating our synthetic images."*

L461-462: "as current instruments cannot make measurements mover both water and land in a limited time and space interval.": I think it would be better to say that the signal-to- noise-ratio is lower over water making measurements more challenging. *"as current instruments cannot make measurements over both water and land in a limited time and space interval."*

565 replace by ". Indeed, the difference in reflectivity between terrestrial and aqueous surfaces results in very heterogeneous measurement quality, and we can see for example on the OCO-3 SAMs partially overlooking aqueous surfaces that the pixels above these surfaces are often filtered."

L463: I thought it was 20 km. Why is it 30 km here?? We are not talking about the city limit definition. Here we are defining

a "city neighbourhood" to estimate the proportion of aqueous surface in the vicinity of the city. We added "For the analysis of

570 this subsection," to clarify our point.

L465-468: I think this should be part of your methodology and not of your discussion of the results because this makes the connection between your model simulations and the real satellite measurements. *This analysis is much less detailed and precise and is mostly an overview to feed discussions. We thus don't think that they should be put at the same level. Furthermore, we think this will confuse the reader and make the objective less clear.*

575 L468: Why 11 degrees? Above, you derived a threshold of 12 degrees. *Error, corrected.*

L471: As can be seen for the cities at the west coast of middle Africa, there are regions with large cloud frequency in Africa. Please rephrase. *This sentence is clearly wrong, we are sorry for this. Replaced ", as cloud cover and spatial variability of wind direction are generally lower in Africa than in other continents" by ". Indeed, for those cities the emission budget is the discrimination criteria, and not the cloud cover nor the spatial variability of the wind direction."*

580 L474: "no more observable cities": Please rephrase because this means that there are no cities that can be observed. You could e.g. write something like "the number of cities does not increase..." *Done*

L476: "if observed daily": maybe better "if there were daily SAMs or overpasses" *changed to "if there were daily overpasses"* L477: Please move this sentence above to around L466 where you describe the general procedure. *moved to 1.460*

L480 and L484: "stand[s] out" is not a scientific notion. Please remove and just write the facts, e.g. "In Australia, only five 585 cities..." *ok*.

L481: "For this contintent": Maybe better talk about the five cities instead of the contintent. ok.

L484-488: I think it would be much better here to talk about absolute number of cites instead of the relative number since the number varies a lot between contintents (e.g. 5 in Australia and 273 in Asia). *numbers added*.

L496: "xx vertical levels" Please include the number. In addition, the vertical resolution in the boundary layer is of relevance 590 here. *Sorry for the typo. The number is 49*.

L497: Do you mean 137 levels? *No : https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-pressure-levels? tab=overview*

L500: "is less sensitive to sampling": I do not understand what you mean by that. For a given grid spacing, you get variability only for a certain resolution for all variables. Please clarify. *Typo. We replaced sampling by resolution*.

595 L518: "precise" What do you mean by precise? How representative are these thresholds for real applications? *We mean that* we have studied they're stability to changes in the datasets and they are stable. The representativness is discuss in section 6.1 and 6.3. The conclusion has been greatly corrected and we have detailed our idea.

L532: But one of the strengths of your method is that you can give some indication which cities can be used for satellite observations. So, which cities come out of your study whose emissions can be observed from space? This conclusion is

600 missing here. The cities are the ones passing the criteria. As the spatial variability of the wind direction may be seasonal and the emission budget might evolve rapidly, we think that putting cities names might distract the reader from the main point of the study. Code and data availability: I don't think that this is conform to AMT policy. Please add your data to a repository to be publicly available. *this will be check with the editor*.

Appendices A and B: Actually, I do not see the reason to put these figures into the appendix of the paper. They can be part of the main text. Their discussion is done in the main text only anyway at the moment. *see answers above*.

Fig. A1: Please add information to the caption how the emissions shown in the panels are calculated. *Addition of "The emissions maps are taken from ODIAC."*

Fig. A1 caption: "OLAM boundaries": Please clarify: Is this your estimated area of the city or is this the GRUMP product
mentioned in Sect. 2.4? If it's the GRUMP product, I would prefer that you show the boundary of the city you use in your analysis. *This is an error. The OLAM boundaries (= Grump limits) were present in a previous version but removed. Removal of " of the OLAM boundaries of the cities and the boundaries"*.

Table B1: As mentioned earlier, I'm missing the cloudiness as a parameter here which will be very important to select times suitable for satellite measurements. *See previous comments*.

615 L547: "in over 98%" Don't these methods vary in this number? Yes. Addition of "for each of the three methods." As this variations is only a few percent, we do not judge it relevant to detail further.

Fig. C1: The quantile for the emission budget is not in the range between 0 and 1. Indeed, there was a typo in the label.

Fig. C1: The maximum true ratio in panel (e) is 5 whereas it is 3 for the retrieved ratio in panel (d). How can you explain these differences? *As can be seen in the figure, the difference is important only for the last decile, i.e. when the anthropogenic*

620 enhancement is high compared to the background variability. We haven't explored this point, as it was not judge sufficiently relevant by the tree learning method, and as the conclusions might not be used with actual data as our modelisation of the noise is simplistic.

Fig. C1: panel (f) please add units of the standard deviation units added.

Fig. C1 panel g: Where does the local minimum at the 0.5 quantile in both methods come from? *This minimum seems to* disappear after filtering and is not judge as an important critera by the decision tree. The values for the optimized radius seem to be driven by two things : the spatial variability of the wind direction and the shape of the city. Given the small number of cities, we think that this pic is due to weird effect of the relationship between the two. Moreover, the statistically-speaking low number of cities does not help to have a smooth curve and increase the chance of having outliers.

Fig. C1 caption: Please add to the caption why there are only 2 lines in panel (g).Caption of Fig. C1: "error" with respect to what? Addition of "The optimized radius shown in panel (g) is a parameter of the gaussian plume models (see section 4.3) and is therefore not calculated for the other methods." The legend says "the error on the emission estimate" therefore we do

not understand the reviewer second comment. We replaced estimate by estimation.

L567-568: This sentence "Cities with emissions..." does not make sense to me. Please rephrase. "important" was missing. Remove typo at the end of the sentence also.

635 L571: Please remove "very" *ok*.

630

L572: Please add more information at which quantiles they are similar. "*is*" changed to "are". Addition of "(typically above the 6th decile)"

L573: Where does the "real" anthropogenic signal come from? Changed to "actual" to match the previous terminology.

L578: Please remove "very" or define its dependence e.g. by numbers. ok

640 L583-586: I don't understand these arguments. From my understanding, if the variables are correlated, only one of them should be included in this analysis in the first place. *We have detailed our purpose in section 4 following similar remarks earlier in the review.*

L590: There is no section 5.3.4.2 reference corrected

L590: There is no table 5.2. reference corrected

645 L592: Why is the number lower for CS and IME? *Those methods seem a bit less sensitive to the spatial variability of the wind direction. We have for example 22 occurrences of just the emission budget as criteria for the CS method.*

L593: Remove "very" here. ok

L598: Again, there is no table 5.2. Please update. reference corrected

L608 and L609: I do not understand what you mean by "standing out". Please rephrase and explain. "without standing out

650 strongly (appears for less than half of the samples)." replaced by "As this criterion appears for less than half of the samples, we do not consider it as sufficiently relevant."

L611: Why do you now use the same thresholds as for GP2? The thresholds will depend on the method you use. In the previous section, you showed that the thresholds are different for each method and to use the optimal one for each method would be the way to go. *We do this to simplify. The differences are furthermore quite thin : they all fall in the spread of the*

655 thresholds found for GP2. We thus think that it should tend to converge with a bigger dataset, more various data. An explanation has been added : "As the thresholds distributions are similar for all inversion methods, we choose to use the same threshold values than those found for the GP2 method".

L611: The description in section 5.2.1 has never been referred to as GP2 method. Please add this to this section. *Addition 1.545* "*The gaussian plume method used in the main body of the article will be now referred as GP2 for clarity.*"

660 Fig. C2: Please add the unit to the y-axisDone.

Fig. C2 caption: Do you mean emissions > 2.1 ktCO₂/h? Yes. Correction made.

L614: What do you mean by "accuracy"? Is it the median or the spread or both? *Spread. Changed to "spread of the error generally decreases with higher cities emissions"*.

1.3 Technical corrections:

665 L28: Please use citep instead of citet *ok*

L29, L37, L38: XCO₂: subscript for number 2 ok

L30: citep instead of citet ok

L59: remove second "the" ok

L61: "is" -> are "errors" changes to "error"

- 670 L83: help to identify *ok*
 - L84: help to identify *ok*

	L88: Remove "The" at the beginning of the line. <i>ok</i>
	L88: move "used" before OLAM simulations ok
	L97: Use (?)or Ullrich citation ok
675	L116: I think, it should be "power plants" ok
	L145: a -> an <i>ok</i>
	L154: 2063 km ² (squared is missing) ok
	L156: Remove comma between "Note that" and "the" ok
	L161: Use ?or the citation citation removed
680	L163: citation is wrong <i>ok</i>
	L201: It would be better to include commas between the vector elements. ok
	L214: annex -> Appendix <i>ok</i>
	Figs. 2 and 3: Please switch the order of the figures to match the mentioning in the text. Early reference to fig 3 was removed.
	The order is now correct.
685	Sect. 4.2.1: Please convert the verbs from future to present, e.g. "will separate" -> separates <i>ok</i>
	Fig. 2 caption: will classified -> will be classified <i>ok</i>
	L294: "are based" \rightarrow is based <i>ok</i>
	Fig. 4: black line -> black dotted line <i>ok</i>
	Fig. 4 caption: the the -> the <i>ok</i>
690	L397: modelisation -> simulation we do not agree with this correction
	Fig. 5: typo in y-axis caption: % of the true emissions <i>ok</i>
	Fig. 6: right panel x-axis: Better "meeting" instead of "combining". ok
	L476: "an order of magnitude of" \rightarrow approximately ok
	L484: "of cities of" \rightarrow of cities with ok
695	L504: "5.2.2" \rightarrow "Sect. 5.2.2" <i>ok</i>
	L511: "XCO ₂ " add subscript <i>ok</i>
	Fig. A1: Please add more space for the Ningbo panel. <i>ok</i>
	Fig. A1: Please reverse the color scale because it is confusing that red means lowest emissions. The plots seemed to us less
	lisible with the inversed colormap suggested by the reviewer. We prefered to keep it that way.
700	Caption of Fig. A1: Add "Sect." to 2.3 ok
	Caption of Table B1: 1first -> first <i>ok</i>
	Caption Table B1: W2D -> W (which actually occurs in the table) No, we are talking here about the wind use for the
	estimation of the divergence, shearness, We agree that the notation was confusing and changed it.
	L538: "optimized" -> "applied" or "investigated" "investigated"
705	L539: "across" -> for <i>replaced by "of"</i>
	Caption of Fig. C1: remove "according" ok

L568: Remove "emissions." at the end *ok* L598: close \rightarrow similar *ok*

Reviewer 2 2

710 The manuscript addresses an important scientific issue and presents an innovative approach to assess CO2 emissions from urban areas. However, many parts in the preprint suggest that it is work in progress. The study holds potential but necessitates substantial revisions to strengthen its clarity as well as scientific rigor.

We would like to thank the reviewer for this complimentary comment. We hope that the corrections made will address his concerns. We have rewritten the introduction and conclusion and added introduction parts to the section and hope that it had helped clarify the article. 715

2.1 **General comments:**

The manuscript should make a clear distinction that its primary objective is not the inversion process itself, but rather the assessment of the confidence in the inversion results via predictable and diagnostic variables. In the methodology section, more emphasis could be put on how the two-step procedure via predictable and diagnostic variables contributes to the accuracy

720 assessment of emission estimates. Indeed, this was missing. We have developped the introduction of this section to make this point clearer.

The manuscript heavily relies on Danjou et al. 2024, which is not accessible for verification. I think this is problematic and impedes a thorough evaluation in parts of this study.

It seems that there as been a problem. The manuscrit of Daniou et al. (2024) was provided to the editor so that it can be send to the reviewers. Please accept our apologize for this. The article has been published in RSE and is now accessible at 725 https://doi.org/10.1016/j.rse.2023.113900.

The manuscript lacks clarity on what constitutes the error. The reference data used for determining the error is not explicitly defined. A definition of the error as been added 1.76 : "As we are working with synthetic data, the error in the emissions estimate is directly accessible by comparing the emissions estimated by the inversion method with the synthetic true emissions used in the OLAM simulations."

730

The manuscript does not provide validation of its results with actual satellite data (e.g., OCO-3 SAM) or ground truth measurements. The absence of this validation makes the reliability of the simulated results vague to some extent.

The use of synthetic data is often used alone (Broquet 2018, Lespinas 2020, Kuhlmann 2019) to validate methods as it gives a good idea of the expected behaviour of these methods. There are indeed always differences between real and synthetic data, and

735 differences in sensitivity will certainly be visible with real data, as there is still much to be understood in XCO₂ measurements at fine scale. Moreover, correlation unreprensented here can also appear that will highlight other criteria. Nevertheless, the criteria found here will still be pertinent with real data, are they will still be driving the error. From our point of view, comparing real and synthetic data (and their sensitivities) merits a study in its own right.

The variability of the error distribution remains significant across different cities. What are the implications for estimations

740 from real satellite images? It means, as stated in the conclusion, that there are still things that we do not understand, despite the progress made by defining these criteria. We have developed the conclusions to answer this question.

The study should discuss the detection limits of current and future satellite missions and how those might impact the results. Is the purely random noise model imposed on XCO2 data in the study representative of real world atmospheric and environmental conditions? In actual scenarios, factors like surface reflectivity of different land types and the presence of aerosols can

745 introduce more structured or systematic errors rather than purely random ones. Would incorporating more realistic, structured errors enhance the model's applicability and accuracy in real-world urban CO2 monitoring scenarios? Given this potential limitation, what implications does this assumption have for future research?

Understanding and simulating the error structure is an active field of research (see Bell 2023 https://amt.copernicus.org/ articles/16/109/2023/, Taylor 2023 https://amt.copernicus.org/articles/16/3173/2023/amt-16-3173-2023.pdf, Worden 2017

750 https://amt.copernicus.org/articles/10/2759/2017/). We think that the complexity necessary to accurately take this into account (as can be seen in the papers cited) is out of scope of this study. Integrating this would only add complexity, increase the error and maybe add some new criteria, but the criteria that we find in this study should still be pertinent.

The selection criteria for the size of the target emission zone radius, are not comprehensively described. I can't find a clear rationale for the chosen size of the emission zone radius. Any potential to estimate this radius through an inversion approach? *Indeed, a clear explanation was missing. We have reshaped the first paragraph of this subsection and introduced a rationale.*

The influence of cloud coverage on satellite observations is a significant factor that the manuscript should address. When it comes to determining which cities are most suitable for measurement, cloud cover is indeed a major issue, and the frequency of cloud cover is an important criterion for city selection. We examined this point in section 6.2.

755

We have reserved this analysis for discussion, however, because realistically adding the effect of clouds in images (filtered pixels and contamination of neighbouring pixels) and trying to objectively quantify their impact on error is of a complexity that would merit a dedicated study to do it more properly than what is proposed in the discussion.

We also believe that, once an image is partly contaminated by clouds, it is not worth processing. Indeed, the effect of cloud presence on the measurement is very complex, due to the presence of 3D cloud radiative effects in OCO-2 retrievals (https://doi.org/10.5194/amt-14-1475-2021). Given the size of these effects (of the order of a few kilometers) and the size of

765 our images (a few tens of kilometers), we doubt the value of trying to obtain an estimate from an image contaminated by clouds. However, this remains to be demonstrated, and the complexity of such a task requires, in our opinion, a complete study and has no place here.

Adding clouds would not alter the conclusions we have reached, the criteria identified should still be important even in the presence of clouds. Thus, adding cloud coverage would only increase the error and add another criterion.

The authors of the manuscript should revise Section 3 to summarize only the key aspects of the Danjou et al. 2024 study that are directly relevant to their current research. As mentioned above, it is problematic that the Danjou et al. 2024 paper is not yet available and that the study heavily relies on it. *Danjou et al. 2024 is now published. We tried to remove the unecessary*

references to this paper and regroup the ones that were unevitable. We hope that this article is now easier to read and less repetitive from that point of view.

775

The description of the OLAM model and its simulations should be more comprehensive in order to better understand the simulation results. *Changes have been made following the specific comments of reviewer 1*.

The manuscript acknowledges that the method is not universally applicable to all cities and is still a work in progress. However, it should also describe how the proposed method would be applied to real satellite measurements and critically assess, whether its applicable at all within the error budget. *We do not share the conclusion of the reviewer. Could the reviewer*

780 indicate which sentences give this impression? Indeed a gaussian plume is applicable to all images and the criteria are also valid for every cities.

The conclusion should reiterate the study's focus on developing a procedure for accuracy estimation, summarizing how the study advances this goal and its implications for future research and practical applications. *We have rewritten the conclusion, keeping in mind the reviewer advices.*

785 2.2 Specific comments

The manuscript frequently uses abbreviations and technical terms without defining them (e.g., XCO2, UNFCC, OCO, ppm, GOSAT-GW, WRF, OLAM, IQR). *definitions added in the relevant places*.

3: The phrase "selecting images to be processed" should be more clearly defined. *changed to "selecting the images to be processed"*

Fig 1: Identifying the factors behind the peak XCO2 values in the simulation domain deyond the city boundaries. *The two small peaks on the east of the city may correspond to an XCO2 enhancement due to the city that as accumulated earlier in the day and is now ventilated. The peak on the bottom of the images seems to be coming from the city at the edge of the image when we look at a more broader view.*

46: The Danjou et al. (2024) should be made available to the reviewers due to its significant relevance to the research. *It should have been. Sorry for this issue.*

53: Clarify local background signal (not clear to me, what is meant by this term). *it is the background signal in the vicinity of the city (please see Schuh 2021 for a more accurate description).*

56, 58: "This study" can be misleading. Write "The study". Changed to "Their study"

48-50: Consider moving the sentence up to line 25, before you start describing the OCOs. *The mentionned sentences have been removed as they weren't bring new informations compared to the ones at l.25.*

261: Set by the user? Do all produce the same value? *The description of the decision tree as be rewritten and we hope that it is clearer now:*

"4.2 Analysis with the decision tree learning algorithm

In this study, we seek to better understand the relationship between the input variables (predictable/diagnostic variables) and the reliability of an emissions estimate. For this, we train an explainable machine learning algorithm to predict the relative error of the emission estimate given some input variables (described in Section 4.3), like the variability of the wind direction or the emissions budget, and then study which variables are determined to be relevant by the algorithm. We choose a regression decision tree for this, as they work by learning simple decision rules and therefore are highly interpretable while able to find non-linear relationships between the inputs and the target variable.

810 *4.2.1 Description of the decision tree learning algorithm*

A decision tree is constructed following a recursive process: at each step, the algorithm splits the data into two subsets following a binary rule on a single variable, finding the split that best reduces a particular loss function on the target variable. Each subset is split further into two until some stopping condition is reached (see Fig. 2 for illustration). This algorithm therefore splits the input space into regions, where each region corresponds to a similar value of the target variable (i.e.

- 815 the error on the emission estimation in our case). We use the regression tree implementation from the scikit-learn library (Pedregosa et al., 2011) with a squared error loss, and impose conditions on the algorithm to prevent overfitting (creating over-complex trees that don't generalise well): we set the maximum depth of the tree to 2 (i.e. two levels of binary splits) and we impose that the leaves must contain at least 10% of the training set. The training set (at the root node) is described in the following paragraph."
- 405-406: Please clarify why Paris exhibits such a low emission rate? Is this due to the absence of significant point sources? Indeed there are no significant point sources in Paris. However we do not think that discussing the low emissions of Paris is relevant in this study, are we are working with synthetic data and are not interested in city in particular.

418: What are the implications or consequences for the study if the dependencies of errors are not completely comprehended, even when using synthetic data. *This study brings objective criteria to evaluate the accuracy of an emission estimation, criteria*

825 that have not been evaluated as precisely until now to our knowledge. The error distribution of the emission estimation has not yet been (and cannot be?) fully characterized. Thus we will still have a non negligeable range of uncertainty on the bias given by an emission estimation for a certain city. However, the criteria found here remain pertinent and will still be pertinent when applied to real data. We have adapted the conclusion to emphasise this.

Fig. 5: Typo in y-label (thrue). *ok*

316: The GP2 inversion method is presumed to be a variation of the Gauss Plume approach. However, at this point it is unclear for me what the '2' in 'GP2' represents. Please provide further details or clarification. *It is a typo remaining from an older version of the draft. There was a GP1 (a variation) that we discarded. We thought we had removed this naming in the main body. It is now done.*

520: Was the 12° threshold for wind variability found empirically or is there a rationale behind choosing it? Is this higher variability threshold, compared to what's mentioned in Danjou et al. 2024, a result of the increased resolution in the model? *The threshold of* 12° *is the one found in section* 5.2 *of this article with the tree learning method. We have rewritten this paragraph of the conclusion and , among other things, replaced* 1.518 "We were also able to determine precise and objective thresholds *on these criteria to select the images.*" by "This analysis with a learning method also provides precise and objective thresholds *to these criteria supporting the selection of images.*"

840 The threshold that the reviewer refers to may be the 7° threshold defined in Danjou et al. 2024. It was empirically defined, which explains the difference. Addition of "(empirically defined)" l.317

578: The error appears to be highly sensitive to the city's radius. Could you clarify what "pseudo-image filtering" specifically entails? I don't have access to the Danjou et al. 2024 source for reference. Additionally, referring to line 550 and following, I guess it implies filtering out scenes with variability above a certain threshold? *This minimum seems to disappear after filtering*

- 845 and is not judge as an important critera by the decision tree. The values for the optimized radius seem to be driven by two things : the spatial variability of the wind direction and the shape of the city. Given the small number of cities, we think that this pic is due to a weird effect of the relationship between the two. Moreover, the statistically-speaking low number of cities does not help to have a smooth curve and increase the chance of having outliers. We rephrase 1.551 and 1. 578 to clarify and make the statements more self sufficient in regard to Daniou et al. 2024.
- 58: What are pseudo-images? Synthetic 2D CO2 concentration images, I guess? yes. Precise definition added l.51 : "synthetic satellite images (i.e. pseudo-images) of XCO₂ concentration generated with a meteorological model". We have replaced every occurences of "pseudo-images" with "synthetic images" for clarity.

229: What is the primary source of error in the emission estimates? Does it originate from the tree model or the GP2 inversion method? *The tree model is not used to estimate the emission but to classify the emission estimates. The main sources of error are the estimations of the background estimation and the wind speed (cf Danjou et al. 2024).*

855

47: Improve the English language in this sentence. It encapsulates the primary motivation of the study and thus should be distinctly emphasized and articulated. *We do not understand what is wrong with this sentence as it seems to us grammatically correct.*

76: The frequent citation of Danjou et al. 2024 for all the "light" methods seems inappropriate. It would be more suitable to refer to the original papers specific to each approach. *It seems that the line given by the reviewer is not the good one. On line* 74, we only cite Danjou et al. 2024 as we say that we are using the same methods as therein. We assume that the reviewer is referring to the paragraph between 1.36 and 51 or the annex. We removed the unnecessary references to Danjou et al. 2024 in this paragraph and we added the relevant citations in appendix c1.

74-79: The logic presented in this paragraph is unclear. It would be beneficial to revise and clarify the content for better understanding. We have completely reshapen and rewritten the paragraph, with some additions to make it clearer : "The objective of our study is to resume the series of analysis from Wang et al. (2018); Schuh et al. (2021); Danjou et al. (2024)

and deepen the evaluation of the conditions corresponding to reliable estimates of urban CO2 emissions using satellite XCO2

- images. To do this, we use a little more than a month of simulations of local XCO2 scenes over large cities. This simulations are generated with the global OLAM model and evaluated by Schuh et al. (2021). We use these simulations to generate synthetic satellite images for the selected cities, and estimate their emissions by applying one of the automated and computationally-
- light inversion methods implemented, tested and optimized by Danjou et al. (2024). By using realistic simulations to derive the synthetic image and using a method independent of the model used for the simulations to estimate the emissions, we take into account realistically the uncertainty in the meteorology, atmospheric transport and background. As we are working with synthetic data, the error in the emissions estimate is directly accessible by comparing the emissions estimated by the inversion
- 875 method with the synthetic true emissions used in the OLAM simulations. The study of the emission estimation error for different

cities and weather conditions aim to support the identification of criteria for discriminating between images, separating those whose processing yields statistically reliable estimates from those whose processing is statistically unreliable."

Sec. 2: Mention that ECMWF ERA-5 product is used for meteorological data. It is only mentioned in line 446. *ERA-5 is only used for the analysis in the subsection 6.2, not before (and therefore not in section 2). l 445 "For this analysis" changed to "For the analysis conducted in this subsection".*

880

130: What is the methodological rationale behind assuming constant emission rates? Do you expect that incorporating dynamic emission rates would significantly alter the study's results or conclusions? We did it for the sake of simplicity. We don't think it will altar the results and conclusions, as mentionned in the discussion (1.425-437)

217-221: Does the observation that all methods yield similar results suggest that the assumptions in the model used to generate the synthetic data might be overly simplistic? *No. It was already the case in Danjou et al. 2024. It is explained by the fact that all method share most of their steps : same way of estimating the plume boundaries, the background concentration. The final step (using a gaussian plume or a mass balance method to estimate the emission) has a minor impact on the overall error (as shown in Danjou et al. 2024).*

Sec. 3: Does this paragraph solely describe the work done in Danjou et al. 2024? Certain statements, like in line 160 "The method used here...", are ambiguous in the current context. Does "here" refer to this study or to Danjou et al. 2024? It may be beneficial to condense the paragraph preceding Eq. (1) for clarity. *Addition at the beginning of section 3 of "The complete description of the inversion method and the details and justifications for its specific configuration and implementation can be found in Danjou et al. (2024). We make the assumption that the configurations chosen in the framework of their study remain optimal for other cities. This assumption seems justified, as the chosen methods for each steps differ from the discarded methods*

895 on objective criteria. This section only gives an overview of the different steps and the adaptations (compared to the reference configuration from Danjou et al. (2024)) that were made in the context of this study." We didn't shorten the part before equation (1) as we think that the informations given here are necessary to have an idea of the inversion method used and understand the changes made compared to Danjou et al. 2024.

217-221: Consider clarifying this point earlier in the document, perhaps where the Gaussian plume inversion (Eq. (1)) is 900 introduced, for better coherence and understanding. *Indeed. It comes much too late. We rewrote the introduction of the article and of the subsection to make this point clear from the start.*