Optimising Urban Measurement Networks for CO_2 Flux Estimation: A High-Resolution Observing System Simulation Experiment using GRAMM/GRAL

Reply to reviewer #1

General comments:

This study presents a study on the placement of a monitoring network based on a process model to optimize CO_2 carbon fluxes in urban areas. The research addresses several critical aspects related to the precision and effectiveness of the proposed measurement network, including sensor quantity and quality, optimal sensor locations, the potential inclusion of carbon monoxide (CO) measurements, and the introduction of temporal correlations into prior emissions. A notable strength of the study is its practical relevance, aiming to inform decisions concerning sensor deployment in real-world urban settings, with Heidelberg, Germany, serving as a case study. This approach has the potential to guide similar efforts in other urban areas, making it of interest to both researchers and policymakers. However, there are a few aspects that could benefit from further attention or clarification in the manuscript. For instance, providing insights into potential challenges or limitations of the proposed approach, such as data availability and cost considerations, would be valuable for readers seeking to replicate or adapt the methodology. In summary, this study constitutes a valuable contribution to the field of urban CO_2 flux estimation and measurement network design. With minor improvements in the clarity of methodology and the consideration of potential limitations, it has the potential to be a valuable reference for both researchers and practitioners involved in urban environmental monitoring and management.
We thank the reviewer for the helpful comments and for acknowledging the relevance of the system for researchers and policymakers. We revised the manuscript providing additional information on the uncertainties and limitations and answer to the specific comments below.

Specific comments:

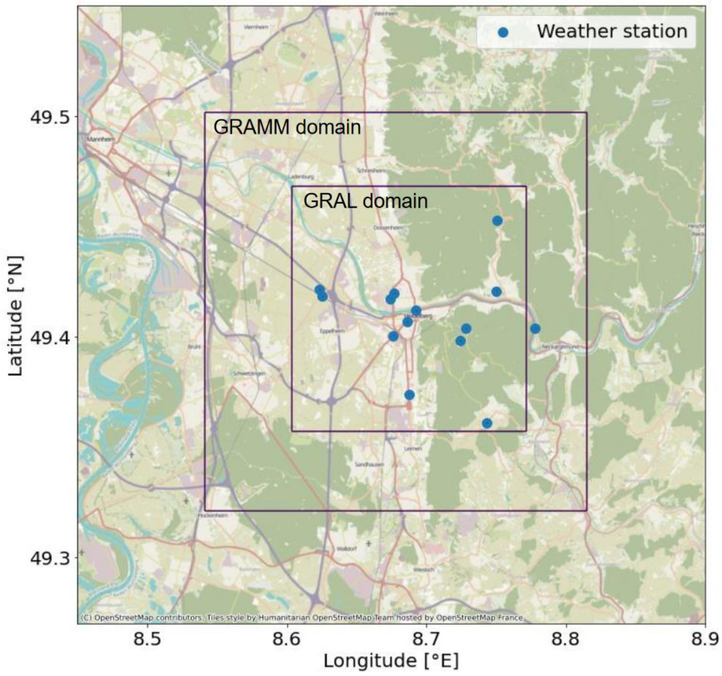
Page 2 and Line 36: Clarity on Observing System Simulation Experiments (OSSEs), When introducing Observing System Simulation Experiments (OSSEs), provide additional context for readers who may not be familiar with this term. Explain briefly how OSSEs work and their role in assessing monitoring networks.
OSSEs provide a controlled and consistent framework for assessing the performance of inversion methods used. In an OSSE emissions as well as atmospheric transport are known. The concentration is obtained by simulating the atmospheric transport of the emissions into the atmosphere. The concentration at selected sites can then be used in an inversion framework to estimate emissions. It is possible to e.g. add measurement uncertainty or model transport uncertainty to the concentration, or to change the prior emissions and evaluate the effect on the emission estimate by comparing to the known true emissions. Therefore, an OSSE enables isolating and analyzing various factors that contribute to uncertainties and errors in emission estimates. We have modified and extended the description and role of OSSEs in the revised manuscript.

Page 2: Consider providing definitions or explanations for key terminology used in the introduction, such as “pseudo observations” and “Jacobian” This will aid readers in understanding the technical aspects of your research.
Pseudo observations refers to the modelled concentration field sampled at selected measurement sites. We obtained the concentration by forward simulating the true emissions using the atmospheric model and adding a model-data mismatch error to

mimic measured concentration data. We have removed the terminology of pseudo observations and explicitly explained it. The Jacobian matrix is a linearization of the forward model representing the sensitivity of the observation to the states. We have added this description. We have read through the paper again and added an explanation where we thought it might be helpful or where it was specifically suggested by reviewer #2.

Line 100: Mentioning that the wind field resolution for GRAL is 2m with a total of 200 cells is informative, but you could briefly explain why this level of detail was selected and how it impacts the model's accuracy or performance.
GRAL has 2m vertical resolution and 10m horizontal resolution. These properties have been chosen following previous studies e.g. by Berchet et al. (2017). 10 meters is approximately the size of a street in an urban area, therefore enabling the simulation of street channeling. For Heidelberg, May et al. (2023) evaluate the model performance with these settings. The paper is under revision in Atmospheric research. May et al. (2023) show that for this resolution the urban meteorological fields can be simulated very well in Heidelberg with small biases and RMSEs in wind speed and wind direction. We do not have any information how a lower or higher resolution would impact the results in Heidelberg.

Consider optimizing Figure 1 by suggesting that the GRAL domain be displayed directly within the GRAMM domain. Also, shows the basic outline of the city of Heidelberg. Additionally, supplement the horizontal and vertical coordinate headings with the units of latitude and longitude, and include a legend.



The GRAL domain was already displayed in the GRAL domain. We have added coordinate headings with unit and included a legend. For clarity, we have decided to leave out the inlay showing emissions and we have not added city boundaries as the urban areas can already be identified looking at the underlying OpenStreetMap and additional boundaries would make the plot more difficult to read. However, note that Figure C1 displays the district borders in the GRAL domain.

Line 202: Explain the significance of using administrative districts as emission groups in your study. How does this choice impact the optimization process, and why were small districts and border districts aggregated?
The choice of state vector is important as it has political, as well as numerical implications. Jungmann et al. (2022) hypothise that providing CO2 information on high resolution may provide policy makers with information, which may enhance ambition and ability for climate mitigation. At the same time, reliable and independent information of emissions on high resolution requires a large number of sensors to constrain the fluxes. Therefore, we chose the administrative districts as meaningful political unit, which can still be constrained with a realistic number of sensor nodes. We chose to aggregate smaller and border districts as they are very difficult to constrain as they contribute only weakly to an overall enhancement. In principle, other choices of emission groups are possible and may be explored in further analysis.

Line 216: TNO Abbreviation: Clarify what TNO represents (if it's an abbreviation).
TNO stands for the Netherlands Organisation for Applied Scientific Research. We have added this in the manuscript. We have also added a Table of Abbreviations to the Appendix.

Line 226: It may be helpful to add a brief explanation of Monte Carlo experiments and the analysis process to elucidate the concept for readers unfamiliar with Monte Carlo experiments.
Monte Carlo experiments are simulations that randomly sample a model variable, in our case sensor location, to estimate the probability of having a certain outcome, in our case of having a certain information content of the inversion. We have added a sentence in the manuscript.

Refine the information on Figure 2 map sheets and ensure that maps include a legend, latitude, longitude, and compass information.
Done.

The discussion of the uncertainty analysis of the overall model development is somewhat sparse and scattered. There is a need for additional integration of the discussion of uncertainty.
We have added a discussion on uncertainty in the new discussion section. We address some important sources of uncertainty including model transport and instrumentation errors, neglecting biogenic fluxes and transported background concentration, as well as the choice of state vector in the inversion framework itself.

Subfigures Numbering: Add numbers and subfigure titles to subfigures in some groupings. For example, Figures 2, 3, 4, and 6.
Done

Modify “a.)” in the figure captions to “(a)” to indicate this, and follow the same format for other subfigures.
Done

I read your paper published in 2015 "Vardag, S. N., Gerbig, C., Janssens-Maenhout, G., and Levin, I.: Estimation of continuous anthropogenic CO2: a model-based evaluation of CO2/CO, CO, δ13C-CO2, and Δ14C-CO2 tracer methods, Atmospheric Chemistry and Physics, 15, 12705-12729, https://doi.org/10.5194/acp-15-12705-2015, 2015." and comments from reviewer Jocelyn Turnbull. I found the comment that the study by Vardag et al.,(2015) suggests that in Europe, CO may not be as available as a tracer of fuel CO2

as it is in other regions due to the low ratio of CO:CO2 emissions from European transportation. In contrast, in section 3.3 of this study, the tracer role of CO is emphasized, especially in distinguishing between different emission sources, such as transportation emissions. However, the fact that transportation emissions are generated from fuels, which includes emitted CO2. there is a need for further clarification or discussion as to what causes this discrepancy.
This is a very helpful remark. Most fossil sources emit CO as well as CO2 in a given ratio. We list the ratios used in a revised Table 1 as there have been a mistake in the previous table 1. We have realized that we used the incorrect names of the GNFR sectors and in few cases miscalculated the emission ratio. Note that the correct values were used in all calculations. We have corrected the table in the manuscript. As one can see, the emission ratio for CO depends very much on the GNFR sector. Even within the traffic emissions (F1-F3) there is a huge spread of different emission ratios. In general, the more distinct (e.g. the higher) the ratio CO/CO2 for a given sector compared to the other sectors, the better the tracer for the sector. Therefore, it is in accordance to Vardag et al. (2015), who state that the quality of CO as tracer for fossil fuel is deteriorating. However, it is still a valuable tracer for fossil fuel as was confirmed later e.g. by Maier et al. 2023 and Kim et al., 2023.

Note also that the study by Vardag et al. (2015) uses mean ratios of CO/CO2 (plus fixed diurnal cycle) and therefore does not consider a variation of CO/CO2 ratio dependent on the area of influence, i.e. on the footprint. This variation complicates a good estimation of fossil fuel CO2. However, in this study we conduct an actual inversion taking into account the area influencing the enhancement at every hour and therefore the emission ratio itself actually varies depending on the footprint. Therefore, the spatial variation of CO/CO2 can be taken into account in this inversion. In the manuscript we already discuss that the inversion result depends on the actual CO/CO2 ratio used. We have now picked this up in the discussion as well.

Note additionally, that we have updated Figure 8 as we previously used the CO/CO2 emission ratio of F1 instead of the weighted mean CO/CO2 ratio of F1-F3 to construct the CO concentration record for traffic as would be correct and as the text in the manuscript implies. Figure 8 now shows the estimation of total CO2, traffic CO2 and combustion CO2, when using the mean ratio for total traffic emissions (weighted mean of F1-F3 about 9 ppb/ppm) for the construction of the CO record. As expected, we see a slight deterioration of CO as tracer for traffic emissions, but no changes in the general picture. No changes in the text of the manuscript were made.

The conclusions section is quite long, and some of its content overlaps with the results and discussion. Consider optimizing the structure of the manuscript, and it is recommended to add a separate discussion section. The conclusions should be summarized insights based on the results of the entire study.
We agree that the manuscript could benefit from separating discussion and conclusion section. We have restructured the final chapter such that we have included a discussion section, in which we discuss the most important results and in which we add a discussion of uncertainty as requested above. The conclusion section now only contains the summarized insights of using GRAMM/GRAL for the inversion.

References in the Reply:

Berchet, A., Zink, K., Oettl, D., Brunner, J., Emmenegger, L., and Brunner, D.: Evaluation of high-resolution GRAMM–GRAL (v15.12/v14.8) NOx simulations over the city of Zürich, Switzerland, Geosci. Model Dev., 10, 3441–3459, https://doi.org/10.5194/gmd-10-3441-2017, 2017.

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Kim, J., Miller, J. B., Miller, C. E., Lehman, S. J., Michel, S. E., Yadav, V., Rollins, N. E., and Berelson, W. M.: Quantification of fossil fuel CO2 from combined CO, δ13CO2 and Δ14CO2 observations, Atmos. Chem. Phys., 23, 14425–14436, https://doi.org/10.5194/acp-23-14425-2023, 2023.

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Vardag, S. N., Gerbig, C., Janssens-Maenhout, G., and Levin, I.: Estimation of continuous anthropogenic CO2: model-based evaluation of CO2, CO, δ13C(CO2) and Δ14C(CO2) tracer methods, Atmos. Chem. Phys., 15, 12705–12729, https://doi.org/10.5194/acp-15-12705-2015, 2015.