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Interactive comment on "Monitoring CO emissions of the metropolis Mexico City using TROPOMI CO observations" *by* Tobias Borsdorff et al.

Anonymous Referee #2

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General comments:

The paper presents the results of a two-step optimization using carbon monoxide column measurements from TROPOMI over Mexico City. The atmospheric model WRF coupled to a city inventory of CO emissions is used to generate response functions for 10 urban districts. About two years of data have been simulated to estimate the CO emissions for these districts. The simulations and the design of the response functions have been carefully constructed. This topic is highly relevant and the use of TROPOMI data to constrain the city inventory is sound. However, the study has two major problems that need to be addressed before publication:

- two-step minimization: The optimization of the emissions requires two steps. The first step (pre-fit) filters out a significant fraction of the TROPOMI data based on several criteria, while the second step (final fit) includes the entire data set. Some of these criteria require more justification, especially when threshold values are bieng used without any justification. But more importantly, this two-step process implies that the same measurements have been used twice. This approach seems to be a solution to the noise affecting the model-data residuals, hence limiting the convergence of the optimization system. In figure 5, there is almost no difference between the pre-fit and the final fit. The results are already constrained after the "pre-fit" step, except that the error bars further decrease, which seems artificial without assimilating additional measurements.

To be clear, data should never be used twice in the optimization as it artificially increases the information content from the data set. Instead, the emissions should be produced by a single optimization procedure, iterative or at once, but extracting information only one time. If the noise is the inherent problem here, it should be treated by filtering out the noise in the data or in the model. Smoothing data signals, decomposing the signals into frequencies, or averaging over time (both model and data) will help extract the information from noisy model-data residuals. Other approaches like Wasserstein distance or other machine learning techniques will help remove the noise. The optimization procedure needs to be revised to produce robust emissions and uncertainties. As it stands, the selection of data is arbitrary and the optimization uses the sae data multiple times.

- Background determination: The determination of the background CO values is never explained in details. The first paragraph of Section 4 describes very briefly that CO background has been fitted. Which domain has been used? The entire State of Mexico? Considering the topography, the gradients over the domain, and the potential contamination by other sources (such as fires, but also cities, industries, shipping, ...), the uncertainty associated with the background determination needs to be quantified and included in the optimization. The uncertainty associated with the background seems to be equal to zero in the final fit (section 3.4). How is the uncertainty defined in the optimization? Zero values appear in the prior error covariance matrix (P7-L14). It suggests that the background is pre-defined (before the final optimization). A section should describe precisely how the background values are determined in (or before) the optimization.

Assuming you provide a coherent one-step minimization procedure, and a robust determination of th background values for each day, I recommend that you include some pseudo-data experiments to evaluate the potential of your optimization to constrain the city emissions. Simple perturbations should be added to urban districts to determine the actual constraint from TROPOMI data.

- As a last comment, the selection of data with low wind speed conditions will increase the model errors. If the aboslute wind speed is 2 m/s, an error of 2 m/s in wind speed corresponds to an error of 100% on the emissions. It maximizes the local enhancements which helps with the large noise, but this filter is typically the opposite in most studies using satellite data (minimum wind speed). Removing noise will help removing that threshold which seems to be a simple but risky solution to reducing the noise in model-data residuals.

Technical comments:

P2 – L1: “and its transport in the atmosphere “: Unclear.

P2 – L20: Add references for the error sources

P2 – L30: “Here the emission estimation changed by 0.42 Tg/yr 30 in only 2 years from 2014 to 2016, due to a change in the mobile emission model from ‘mobile‘ to ‘moves‘.” This means that the emission model changed and not the emissions. Has this change been confirmed or validated by other data?

P4 – L5: “The inventory is time dependent and accounts for the diurnal, week-to-week and monthly variations of the emissions” How accurate are these cycles? Considering the overpass time is fixed, the mismatch can be explained by a difference in diurnal cycles in and out of the city. How was the inventory constructed? Does it include traffic counts? Are the other sectors using temperature-dependent relationship?

P4 – L29: "Here, z is the mean elevation in the TROPOMI CO ground pixels and zref = 2240 m the reference altitude which is set to the elevation of Mexico City." This correction is unclear. The altitude used by TROPOMI is defined as a surface pressure. The altitude error depends on the difference between the WRF surface pressure and the TROPOMI surface pressure. Why using an average altitude of Mexico City as a reference?

P5 - L4: "local enhancements of CO are due to emissions of the city districts of the same day" Have you tested that assumption? Basin cities are often problematic with low wind speed for days, which can accumulate signals from more than one day in the basins (example: Los Angeles during Winter). An averaged wind speed or residence time of tracers would help justify this assumption.

P5: Use the current notation for multivariate regression used in most publications (observation operator H, state vector x, prior error cov B, Obs error cov R, observations y, Kalman gain K).

P6 - L17: "with little forward model errors". Unclear. Re-phrase.

P6 – L24: "for low wind speeds more reliable". The model errors are critical during low wind speed conditions when a slight change in wind speed can affect the magnitude of the observed enhancements. Typically, high wind speeds should be avoided because local enhancements are weak while low wind speeds should also be avoided when a small change in the wind speed can significantly change the local enhancements.

P6 – L30: "fit residuum â§Íδâ§Ï < 8ppb, and the standard deviation $\sigma(\delta)$ < 8ppb to limit the effect of too large forward model errors." TROPOMI is an averaged enhancement over a grid cell. Point sources will be under-estimated in the data as the plume will not be mixed over the entire grid cell. This bias has been presented by the TROPOMI

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team. Can you conform the relationship between point sources over the domain and the location of these high model-data differences?

In addition, removing noisy pixels will artificially decrease the uncertainty by removing undesirable pixels. Some of these large model-data differences might be real transport errors or observation noise.

P7 – L1: "$\sigma(\delta)/\delta$(ymeas) < 0.65 to ensure that the forward model can explain the variability of the measured CO field." This value seems arbitrary. How did you define it?

P7 – L4: What I the impact on the seasonal distribution? Does it remove data evenly over the year? This filters are likely to bias your results over specific season. A figure showing the time depencen of the filtered data is needed (or statistics)

P7 – L15: "αbg and αelv are not regularized" How can you optimize the emissions without regularizing the background values? Are they pre-determined? How were they defined?

P7 – 15-20: The balance between prior information and data constraint is usually computed with the Chi2 normalized distance. A value near one will define the optimal balance between the two. Michalak, A., Hirsch, A., Bruhwiler, L., Gurney, K., Peters, W., and Tans, P.: Maximum likelihood estimation of co- variance parameters for Bayesian atmospheric trace gas sur- face flux inversions, J. Geophys. Res.-Atmos., 110, D24107, https://doi.org/10.1029/2005JD005970, 2005.

P7 – L21-24: This approach weighs toward pixels that are co-located with the sources. In other words, it selects preferentially the pixels above the city. In general, it should work but an evaluation perido would be helpful (with and without the filter) to measure the impact of the selection. This approach might bias the results if the model under-/over-estimate urban pixels.

P7 – L23: "temporal variation of the INEM emissions to be about 40% [. . .] vary with 60% around their average" How do you define the 60%? The link between 40% and

60% is not explained. In addition, temporal variations and mean emission errors are not supposed to scale together. This part needs to be described more carefully. The emission errors should depend on the emissions alone instead of their temporal variability.

Figure 4: This figure provides illustrations but is not very helpful to prove that the WRF model is reliable or good enough. Instead, model-data mismatches should be presented in a synthetic figure, for different times of year, using whisker boxes. Snapshots for four days out of 160 is too few to convince the readers. This figure should be replaced.

P8 – L18: “This clearly shows that regional models like WRF have a great potential for the interpretation and analysis of TROPOMI data.” No, this does not demonstrate the model capabilities nor the ability fo the model to extract emissions. Re-phrase.

P8 – L21: “For atmospheric conditions under high wind speeds the WRF simulations can deviate more from the TROPOMI measurements as shown in Fig. 4 (c).” This single day is too limited to conclude anything. More statistics on windy days are needed to prove your point is valid here.

Figure 5: The modeled and observed XCO should be presented first, summarized for the days available before and after filtering. Do the residuals show a seasonality? The results of the optimization are difficult to interpret without the evaluation of the initial model results.

P9 – L1-6: Large model-data mismatches are expected from observations, model errors, and prior errors. If observations are being used twice (if I understood correctly), mismatches will decrease automatically. Optimization should never be performed a second time with the same data. Unless I misunderstood the approach (different data are being used between these two steps), only one step should be performed. Otherwise the constraint from the data is over-estimated.

P9 – L7: “Furthermore, non-uniform variation of the background CO concentration can be a additional reason for this scatter (as shown in Fig. 3).” How did you determine the background? How do you separate the contribution from the city emissions? Is it all performed within the inversion? If so, how do you define background uncertainties? Some additional tests should be performed. If you introduce a background in the bias, is your optimization system able to recover that bias?

Figure 6: statistics should be presented for the entire data set and not only for four days.

P9 – L13-14: “the averaging kernel shows that the Final-fit inversion is insensitive to deviations of the Tulancingo emission from the prior estimate. Whereas the Pre-fit inversion estimates very small emissions for this district, the subsequent regularization changes the emission only marginally.” This is the direct consequence of performing an optimization with the same data twice. Some of the constraint has already been introduced in the emissions.

Specific comments: P6 – L15: “depends crucially” = highly depends on

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