Interactive comment on “On biases in atmospheric CO inversions assimilating MOPITT satellite retrievals” by Yi Yin et al.

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General Comments: This paper aims to evaluate the representation of the CO fields obtained from the assimilation of MOPITTv6 total column (XCO) retrievals (one experiment) and several modelling sensitivity tests. The set of parameters from those sensitivity tests includes the use of posterior emission fields, OH fields, and transport through different grid spacing's, boundary layers and convection schemes.

Further research is needed in some studies using data assimilation to investigate, quantify and in fine understand biases from satellite retrievals, model simulation, and potentially from the assimilation methods (observation operator, error characterization, state vector choices). The comparison of analysis/posterior products can provide a different perspective for the nature of those biases, different from instrument valida-
tion and model evaluation by itself. In addition, the use of different and independent datasets is usually informative about the quality of the assimilated and/or posterior model fields. However, the paper's objectives, methods and conclusions need stronger clarifications. In other words, the conclusions can be misleading with regards to the scientific methods used. The authors should either review their conclusions or consider another evaluation approach before publication.

From the conclusions/abstracts, it is stated that the “purpose of top-down estimates of CO emissions, in which the model cannot directly correct vertical model biases, it is more robust to assimilate the column than a particular pressure level retrieval, a partial profile [...]”.

As it is known, assimilating total columns presents some advantages. For instance, total columns can have lower instrument biases. For pragmatic reasons, it makes sense and I agree that if the observation does not give any information about the vertical distribution, it is more appropriate to not correct for the vertical distribution within the assimilation scheme. However, those conclusions are surprising with regards to the actual work that has been done in the paper. There are no tests that would rigorously test the hypothesis of choosing a method versus another. In addition, some comments are contradictory.

One important point to consider is that assimilating total columns relies on the vertical profile given by the model, thus, it is just the total column abundance that is shifted. Within that framework, there is no reason to expect improvement of the vertical profile, because it means that the modelled vertical profile is assumed to be perfect (relatively to the satellite observation). Or it can be assumed that it is far to be the case in global models (with coarse resolution in both vertical and horizontal). It is also acknowledged in the paper: “From the CTM perspective, the evaluation against aircraft measurements reveals significant model errors in representing the vertical CO gradient, in particular over the ocean.”
Moreover, those errors persist after optimizing emissions, which means that chemistry and transport are both important. This is also acknowledged in the paper, but in the abstract, it is mentioned that: “Consistent negative prior biases to all types of observations in all sensitivity tests suggest an underestimation of current surface emissions in the Northern hemisphere. In contrast, prior simulations fit the surface air sample observations well in the Southern hemisphere but underestimate CO in the free troposphere and on average in the column.”

For instance, Stein et al. (2014) demonstrated that the northern hemisphere spring cannot be attributed to direct CO emission alone. Myazaki et al. (2015) with a simple sensitivity test, a change in the CO + OH reaction rate were able to considerably reduce this bias. These studies suggest that this bias is likely to occur due to a combination of errors from chemistry, deposition, direct and indirect emission processes (vertical distribution, time profile), as well as transport. Far from the sources (in the free troposphere, over the ocean, in the southern hemisphere), it is even more likely that the problem will be due to transport and chemistry (secondary sources of CO and/or the OH sink). In particular, biases can be shared through the CH4/CO/OH system, as Strode et al. (2015) and Elshorbany et al. (2016) posit. In general, please consider discussing those previously published results with regards to the setup used in this study, which presents some advantages, but also some drawbacks to compare and contrast different possible approaches.

In order to improve the study please consider the following: 1. If this paper is aimed to evaluate the impact of assimilating either the profile or the total columns, this can be done using data assimilation experiments together with observation space diagnostics, see El Amraoui et al. (2014). The use of innovation statistics (and data assimilation) diagnostics allows to quantify the bias, while taking into account error variances from both model and observations. In particular, looking at those by Åst Assimilation of total columns and evaluation of profiles (in observation space) Åst Assimilation of profiles and evaluation of columns (in observation space)
By doing this the diagnostics for the assimilated and non-assimilated observations can be run for each case to verify the consistency between the columns and the profile in the observation space. In a case where assimilation parameters are correct (with regards to those same diagnostics) and underlying assumptions are not too violated, it would give a more robust estimate of the impact on the total columns while assimilating profiles and vice-versa.

2. Other studies that aim to improve the model error representation in chemical data assimilation (e.g., Gaubert et al. 2016; Emili et al. 2016 and reference therein) as well as potentials from strong constraint 4D-Var (e.g. Trémolet 2006) could be discussed and analyzed.

3. The assimilation of compact phase-space retrievals (CPSRs) could be considered, which is an alternative approach to profile assimilation (e.g. Mizzi et al. 2016).

4. Thanks to the comparison to HIPPO measurements, the first identification of an upper tropospheric bias last from the MOPITT V4 (Deeter et al. 2010). The identification of the bias and update of the statistics against HIPPO has continued since then (Deeter et al., 2013; Deeter et al., 2017). You can review Martínez-Alonso et al. (2014) for another evaluation of MOPITT profiles and satellite data. Jiang et al. (2013) suggest not to assimilate the profiles in the upper troposphere while Jiang et al. (2017) propose a latitudinal bias correction. There is evidence that errors can arise from the multispectral retrieval for the nighttime oceanic scene (Worden et al., 2010).

5. Finally, please consider to include an extensive discussion on the sources of model error and limitation of the setup of the simulations. You can provide more quantitative results. To do so, it is highly recommendable to use conservative measures to compare simulations such as atmospheric burden for CO abundance and RMSE (or absolute errors) for comparison of simulation with observations. On the spatial resolution, one can also discuss the fact that emissions estimates would be different at higher resolution. The change of resolution changes the distribution of emissions and
thus chemical regimes. The errors evolution with regards to spatial grid spacing can be not linear in chemical transport models. Here, the emissions have been optimized at lower resolution, this leads to serious limitation to conclude about the effect of spatial resolution.

6. Perhaps, a further discussion on the limitation of the methods is needed, knowing that emission is not the only error source. For instance, there is dry deposition (Stein et al. 2014), time evolution coupling and feedbacks of chemistry (Strode et al., 2015; Gaubert et al. 2016; Elshorbany et al., 2016) and vertical transport, the aggregation of VOC's oxidation in one term (e.g. Jiang et al., 2015 and reference therein), etc.

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Specific Comments:
There are some sentences starting with “It seems” followed by a strong fact statement: “The choice of the prior OH seems to produce the largest differences in the simulated CO concentrations at a global scale.” “representing the vertical profile correctly seems to be a grand challenge.” This is confusing, please choose between hypothesis or fact.

The Section “2.1 MOPITT satellite retrievals of CO total column and vertical profiles” is not clear and contains errors. It needs major revision. Can you merge with section 2.4.4? I don’t think the authors should presents the retrieval algorithms. Please provide instead the way they applied the averaging kernels for the columns (equation 1) and the profile (equation 2).

From Yin et al. 2015, it is stated that the MOPITT observations are average on the coarser grid. For a fair comparison, the evaluation should be done at ‘higher’ resolution, note that high resolution for a simulation at 1.895 by 2.5 degrees is misleading. A comparison of the impact of the vertical grid spacing should be done first, what is the observation error differences between low (2.5°x3.75°) and medium (1.895 by 2.5 degrees)? What is the differences in biases?

Minor Comments
Abstract
Page 1, Line 16: “Carbon monoxide (CO) inverse modelling studies have so far reported significant discrepancies between model concentrations optimized with . . . (MOPITT) satellite retrievals and surface in-situ measurements.”
In my opinion, this first sentence is misleading and is not fair to MOPITT itself. It is common in atmospheric composition that there are discrepancies satellite and surface observations, or between satellite themselves (Kopacz et al. 2010). It usually leads to large improvements in particular for the well-known northern hemisphere spring bias. Which means that the errors are also due to model and coarse resolution. There have been issues in the Southern Hemisphere, but the reasons are not clear. The model errors appear to not be driven by CO emission alone (e.g. Fisher et al., 2015).

1 Introduction

P2, L76: “with most CTMs showing negative biases to surface and satellite observations in the Northern hemisphere when prescribed with current emission inventories (Naik et al., 2013; Patra et al., 2011; Shindell et al., 2006).” The Patra et al.’s study is about TransCom-CH4 and the paragraph is CTM’s biases in Northern Hemisphere spring of CO modelling, please change this reference to Stein et al. (2014).

P2, L85: “MOPITT-based atmospheric inversions were also shown to be biased high when compared to independent in-situ surface observations in the boundary layer (Gaubert et al., 2016; Yin et al., 2015).” Gaubert et al. (2016) showed that assimilating MOPITT improve the CO values at the surface (not the opposite). The cross-validation with FTS in the southern hemisphere suggests that the model has actually a good prior for wrong reasons, the assimilation improve correlation and suggest an underestimation of biomass burning emissions. Please be more precise, at least indicate that it is in the southern extra-tropical region.

P3, L107: “In section 3, we first evaluate the model with MOPITT XCO that is used for assimilation, then […]”. Please clarify, only one simulation is done with assimilation of MOPITT XCO, what is the model?

P4 L152: change “coverting” to converting

P4, L186: “HR2 corresponds to the version called standard physics (SP) in (Locatelli
et al., 2015), where more detail regarding these configurations are described.” Please rephrase, e.g. “The latter corresponds to a version called standard physics (SP), presented in Locatelli et al. (2015), where more details about these configurations are described.”

P5, L189: Please rephrase, “as suggested by Radon […]”, to “as suggested by the comparison with Radon […]”.

P5, L191: Please rephrase “For all versions of LMDz-SACS here”, For all the different LMDz-SACS configurations presented in this study: […] boundary conditions and horizontal winds […].”

P5: L214: “One scale factor is applied to the HR results over the globe to conserve the global mass budget to be consistent with the reference version MR.” Can you explain and be more explicit? If the 3D fields of Formaldehyde have been simulated using different spatial resolution, why would not you keep a different field? Which budget (CO or HCHO)?

P6, L269: “It is noted that the MOPITT NIR/TIR retrievals, combining information from both TIR and NIR, have generally higher sensitivity to the lower troposphere compared to TCCON.” Please rephrase, add a reference?

P7 L305: “Individual aircraft profiles are assigned to certain model grid points given their geographic location and pressure levels, and all measurements are then averaged per model grid point at a 30-minute resolution to compare with corresponding model value.” What would be the impact of spatial resolution? This comparison is in favor of the coarser resolution, why don’t you interpolate to the observations?

P7 L327: I do not understand this statement: “the total column of the model state integral is always conserved to compensate uncertainty from vertical resolution change on the CTM side.” Again, the evaluation at lower resolution is in favor of the coarse run.

P8 L341: Typo, “of the model version or of the OH field”
P8 L345: change “for both OH” to “for both OH fields”.

P8 L350: “It is noted that although we optimize OH together with surface emissions, the system only scales slightly the big-region OH state vectors (in total six big regions over the globe) and thus the inverted surface emissions are sensitive to the prior OH fields.” With OH driving the CO sinks (90 %), how would it be possible to not be sensitive to the prior OH field?

P8 L350: “with the range showing 1-sigma standard deviation of the mean biases of all model grids, the same applies hereafter if not specified otherwise”. Please remind the time period, a large variability is expected for the northern hemisphere spring. P8 L365: “The CO surface sources are conserved in global mass between different resolutions when emitted to the atmosphere, but with the change in resolution, the CO sink via the reaction with OH (associated with different resolutions) may differ.” What is the purpose of changing the resolution if you forced to value to be equal to the coarse resolution? Those differences are what can be interested in this study, because you are comparing simulation with different spatial grid spacing.

P8 L370: “The difference between the HR and MR XCO results (∼1.5 ppb) is of a much smaller magnitude than the differences between the prior and the posterior MR simulations (∼10.4 ppb); it is also of a smaller magnitude than that induced by the two OH fields in the prior forward simulations when the CO sources are identical (∼2.8 ppb for global average with some cancelling effect between the NH and SH). The differences in modelled XCO between HR1 and HR2 are not significant at a global scale.” To remove cancelling effects, could you use RMSE for comparison with measurements, and/or tropospheric abundance (tropospheric mass) for the comparison of different simulations.

P9 L388: “They also slightly overestimate XCO in SH, resulting in a smaller positive bias 2.5±3.1 ppb using INCA-OH (3.0±2.2 ppb using TransCom-OH).” Please rephrase.

P9 L422: “when other setups being the same; here, the 1s standard deviation showing
the spread across prior/posterior simulations and between the two HR models.” Please do not use the average difference, is it with adjusting emissions and chemistry. You could also do a simulation with full chemistry and updated emissions.

P10 L430 and Figure 3: What are the different points, is it the latitude band or the time period (Months)? A large seasonal cycle is expected (see https://www.esrl.noaa.gov/gmd/ccgg/globalview/co/co_intro.html).

P10 L449 and P10 L469: title 3.4.1 MOZAIC measurements over large airports What do you mean by large airports? Did you actually select airports that are larger, in size, in number of flights?

P10 L455: “are larger in the NH than in the SH, consistent with the different in prior model” Please correct to ‘differences’ or ‘different priors’.

P11 L511: “Such bias in representing the oceanic vertical profiles suggests error in the vertical distribution of CO source/sink over ocean or in the vertical mixing.” Please rephrase, there are errors (plural) from both chemistry, horizontal and vertical transport, ocean is repeated twice.

P13 L600: “The choice of the prior OH seems to produce the largest differences in the simulated CO concentrations at a global scale.” It is confusing, please remove ‘seems’, or you can say “Our study shows that the choice of...” Again, do not forgot that having a prescribed OH is a strong approximation (limitation), see for instance (Elshorbany et al.; 2016)

P13 L615: “The North-to-South gradient in TransCom-OH is also closer to a recent observation-derived near equal N/S OH distribution (Patra et al., 2014)”.

I think those two studies are related, the TransCom-OH field is from ACTM_0.99, which is designed to have a near equal N/S OH distribution. You can mention this in the introduction, it is supposed to be the best fit to Methyl Chloroform.

Acknowledgement Most of the acknowledgement are not respecting the recommen-
dation, please consider contacting the instrument PI’s. For instance, the MOZAIC ac-
knowledge (if not updated since) should be as follow:

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Table 1: “List of simulations in this study”, -> ‘list of simulations done in this study’ or
‘list of simulations’.

Table 2: “reference” to “references”

Table 3: How are calculated the error bars (more or less)?