Reply RC1 (DOI: 10.5194/egusphere-2024-632)

Summary
This study investigated the superobservation methodology for satellite observations, especially for chemical tracers. The paper discussed how to construct superobservations and appropriately set their uncertainty. The authors took several aspects into account and visualized their contributions to the resulting superobservations. They also performed data assimilation experiments and showed that their superobservation methodology resulted in improved forecasts compared to simple thinning.

The paper appears to align with the scope of GMD and may have significant implications for data assimilation studies involving satellite observations. Unfortunately, certain points were not clear to me and could benefit from clarification prior to publication. In addition, the paper's readability was somewhat challenging, possibly due to its unconventional structure. Therefore, I would like to recommend Major revisions.

> Dear reviewer, we would like to thank you for your time, effort and well substantiated comments. Below our reply to your comments, we have tried to incorporate as many of your suggestions as possible. We are in particular committed to improve the readability of the paper. All line numbers in the reply refer to the revised manuscript.

Major comments:

1. Clarifications required
Several statements in the manuscript were unclear to me. Most of them could be my misunderstanding, but I would like to ask the authors for enhancing the clarity.

Lines 196–197: The sentence beginning with "Given the same uncertainty," is confusing. Could this be re-written?

> Due to changes in the structure of the paper this point has been moved to the introduction on line 85-88. The sentence has been rewritten to:
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> "If all individual observations with their individual uncertainties are assimilated in a model with a coarser resolution than the satellite, this leads to low-biased analyses, because more weight is given to low observations with a small uncertainty. With the superobservation approach described in this paper, such persistent low biases are largely avoided."

Lines 322–323: Unfortunately, I could not understand this sentence. A rewrite may be necessary.

This sentence and the previous sentence (lines 320-321) have been rewritten to:

“Any systematic error on the slant column also influences the quantification of the stratospheric error discussed in the previous section because the slant column is assimilated for the quantification of the stratosphere.”

Lines 510–511: This sentence was confusing. I guess this sentence compares Figures 12a and 12c, yet I could not find clear differences between these figures.

The difference between the figures is subtle, but systematic. To make this more clear we rewrite lines 493-499 to:

“The regular superobservations and the uncertainty superobservations are similar. Both give a realistic low-resolution representation of the original satellite data. But, as expected, the uncertainty-weighted superobservations have systematically lower values because the weights favour the smaller columns, though the difference remains subtle. This is most clearly observed above Paris and North Africa. On average the uncertainty weighted superobservation in Figure 12 have a tropospheric column of 22.4 μmol m^{-2}, compared to 23.0 μmol m^{-2} of the normal superobservations, which is a reduction of 2.7%. Over polluted areas with a tropospheric NO2 column over 30 μmol m^{-2} this reduction is 5%.”

Lines 561–562: Why does an increase of covariance inflation result in a larger O–B?

Inflating the covariances increases the spread in model results, which in turn impact the analyses. The analyses with an increased covariance inflation produced a lower quality forecast. This can be expected because a too large ensemble spread can degrade the comparison against observations. On the other hand, if the spread is too small, an increase in the inflation may lead to a reduction of the departure.

To clarify this, we add the following changes to the text on line 553-554:

“The increase in spread from the covariance inflation results in a poorer forecast.”

Line 641: What does correlation length mean? The cutoff radius of localization?

In this case the correlation length refers to the spatial correlation lengths introduced in the modelling of the background (forecast) coveriance matrix **B**.

To clarify this, we replace the sentence on lines 640-642 by:

"Data assimilation implementations typically introduce spatial correlation lengths covering multiple grid cells in the modelling of the background (forecast) covariance matrix **B**."

Line 703: I am not sure why adding one improves the results. I understood that N > Neff but does this sentence mean N–Neff=1? Could you explain? Furthermore, I could not understand that "This is not consistent with the experimental data" in Fig. 8c.

Because $N_{eff} < N$, there will always be a point where $N_{eff} * f < 1$. Normally this does not happen because you have at least one observation n. And for n=1 the systematic solution should be equal to the random solution because the sampling method is still the same. Yet for the coverage where N*f = 1, $N_{eff} * f < 1$, this yields an n lower than 1. Resulting in $\sigma_{re} < 1\sigma$. Experimentally this never happens and conceptually this should also not happen. Adding the plus one was a simple way to address this problem, while keeping a continuous function. Based on other comments we have decided to rewrite the section on the representation error. In this rewrite we have more formally derived the need for adding a plus one, which can be found in appendix B. This derivation results in a slightly different formula. Note that in the new derivation the plus one is already added in the random representation error formulation to address problems with the use of fractional observations. This solves the above problem before it occurs

2. The structure of the paper

The manuscript does not have a typical structure that contains an introduction, method, result, discussion, and summary. Although the motivation of the study should be clearly noted in the first section, section 3 explains the motivation of superobservation as well. While section 5 discussed contributions of three aspects on uncertainty, section 6 revisits the topic of uncertainty. I might misunderstand, but I would like to ask the authors to re-consider the structure of the manuscript. This could make the paper more concise.

Because of the nature of the study where the method is our result, we found a more typical structure did not fit the contents, which is why we decided on using an unorthodox structure. But not following a traditional structure does carry additional risk in terms of understandability, thus we appreciate the feedback on this topic. To improve the readability, we have merged section 3 into the introduction. Point 1 can now be found on line 44, point 2 on line 74, point 3 on line 84 and point 4 on line 83, point 5 on line 83 and point 6 on line 89

While both section 5 and 6 discuss the superobservation uncertainty, the sources of the uncertainty are different. Section 5 addresses the dependence of the superobservation uncertainties on the uncertainties of the individual satellite retrievals and spatial correlations between these errors. Section 6 discusses the representation error which is not linked to uncertainties in the individual retrievals but to an incomplete sampling of the grid box. These require a fundamentally different treatment and keeping these separate improves the readability of the paper.

Minor comments

Line 92: Remove an extra "observational?"

We have removed the extra observational

Line 238: Does the left-hand side correspond to ds?

This is correct, we have added this to formula 8.

Line 246: Does A_S mean the superkernel?

Yes, for clarity we have added As to line 242.

Line 299: What are Θ and Θ_0?

These are the viewing zenith angle (VZA) and the solar zenith angle (SZA) respectively. This has been added to the text in line 289 for clarity.

Line 531: I would recommend explaining the experimental settings a bit more. It would be better to include what observations were assimilated, how long the assimilation window, how localizations were set, and how covariance inflation was achieved.

We add the following information on the experimental setting to the text on line 516:

"The assimilation was performed with 32 ensemble members and a two-hour assimilation window. Covariance localization was applied based on species-dependent localization scales, that were derived from sensitive tests in Miyazaki et al. (2012b). Covariance inflation was also applied by inflating emission factor uncertainties(ie. ensemble spread), to a minimum predefined value. Additionally, a multiplicative covariance inflation of 7% was applied to the concentrations. In addition to NO2, the assimilated measurements included total columns from the thermal-infrared (TIR)/near-infrared (NIR) band of the Measurement of Pollution in the Troposphere instrument (MOPITT) (Deeter et al., 2017), OMI SO_2 planetary boundary layer vertical columns(Li et al., 2020), and Aura Microwave Limb Sounder (MLS) O_3 and HNO_3 profiles(Livesey et al., 2022). To demonstrate the impact of different superobservation settings the following 4 sensitivity runs were done for July 2019, only varying the NO_2 observations:"

Line 551: The X^2 metrics seem similar with the consistency ratio (Dowell and Wicker 2009, 10.1175/2008JTECHA1156.1). Are they the same?

The consistency ratio is very similar to the X^2 metric. Both serve the same purpose of assessing the balance between uncertainties and innovations. One crucial difference is that for X^2 the innovation ends up in the numerator while for the consistency ratio it is part of the denominator. As a result, they are like each other's inverse.