Interactive comment on “Reconciling differences in stratospheric ozone composites” by William T. Ball et al.

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1 General comments

1.1 Relevance

It is an inherently challenging task to estimate the magnitude and the patterns of the uncertainties in a data record constructed from measurements by various instruments. Yet succeeding in this endeavour is crucial when the strength of the geophysical signal of interest is similar to the level of uncertainty in observations. The determination of trends in stratospheric ozone observations is a textbook example of this challenge, one that has caused a lively debate within the community over the past few years.

Discussions revolved not only around how to quantify the uncertainties in the data sets and how to incorporate these in the analyses, but also around the regression methods used in time series analysis. This paper proposes alternative methods that are of immediate interest to the ozone community. And to the broader atmospheric community as well, since inferences of climate parameters are often based on (a set of) composite observational data records.

1.2 Methods

The authors adopted a series of techniques to exploit the information contained in four merged data sets to arrive at the probability density function of ozone at each time step, which is then analysed for long-term background trends. To my knowledge, each of these techniques has only rarely or not been applied to ozone data so the results of each sub-analysis is interesting in its own right.

First of all, the singular value decomposition analysis results appear to improve existing estimates of uncertainty in the four ozone composites. I encourage the authors to release these uncertainty estimates, since these are relevant to users of the composites.

Then, this information is used by a particle filter, a sequential Monte Carlo algorithm, together with the transition probability from one month to another extracted from the data. Ball et al. build a convincing case that the particle filter is indeed fairly robust against known or—in some cases—previously unidentified deficiencies in individual composites. Various illustrations show the ability of the particle filter to either adjust for a sudden jump and/or temporary drift, or, to inflate the uncertainty when the information contained in the ensemble is insufficient. The algorithm also unravelled issues not known beforehand, which shows its potential as a tool to improve the considered data sets.

The paper ends by a discussion of the limitations of traditional linear methods in
analysing ozone time series and the authors apply the non-linear method proposed by Laine et al. Doing so brings the lower stratospheric trends from different hemispheres in better agreement and the results seem more stable in the tropical middle stratosphere as well.

1.3 Presentation

There is a vast amount of information in this paper. Perhaps a bit too lengthy in some places, so some trimming here and there (mainly in Section 3) could improve the paper. But overall the authors succeeded in delivering an easy to read, detailed yet fairly concise account of several novel methods and results. I also appreciated the effort they have put into the graphics and the appendix, which contains an abundance of useful and instructive supplementary material.

1.4 Conclusions

I commend the authors for their research and this paper, which is highly relevant to a broad atmospheric research community. It surely fits the scope of ACP and I recommend publication once the minor comments below are addressed.

2 Minor comments

- l.142, p.5: There is still a few % diurnal component between 1-5 hPa which will alias into the long-term trend for uncorrected measurements from instruments on drifting orbits. Please clarify that diurnal variations are not entirely avoided, only those with largest magnitude above the stratopause.

- l.172-177, p.7: I doubt an uninformed reader will grasp the message in “[…] C3 SBUV-MER considers only one data set at a time […], while SBUV-MOD averages overlapping data to combine them […].” A slightly more verbose description of the SBUV-MER merging approach may make the difference with that of SBUV-MOD clearer.

- l.222-223, p.9: Not all occultation instruments retrieve O3 number density on altitude levels, only the UV-VIS instruments do so (SAGE-II). IR occultation missions (HALOE, ACE-FTS) retrieve O3 volume mixing ratio, some even on pressure levels. Please correct this statement.

- l.352-362, p.13: What’s the rationale for the factor 2 increase, and how sensitive are the Particle Filter results to this choice? Over what timescale is the uncertainty expanded? Just the month following the change or is it smeared out over a number of months?

- l.368-369, p.13: How prohibitive is the assumption of uncorrelated measurement errors for the joint-likelihood function? The bottom row of Fig. 4 clearly demonstrates the correlation of the uncertainties in time and between composites.

- l.377-379, p.14: Assuming that $\beta = 10\%$ of the observations need a blow-up of their uncertainty by $\gamma = 100$ is quite harsh. I would expect smaller values for $\beta$ and especially for $\gamma$, whose effect would be to reduce the tails of likelihood. But perhaps your choice is more of a worst-case scenario? How sensitive is the Particle Filter outcome to the choice of $\gamma$ and $\beta$?

- l.403-413, p.15: It should be mentioned here that no transitions were used when an instrument changed. This relevant information is now hidden in the caption of Fig. 5.

- l.440, p.15: I had to wait for 43 lines to find out how large N is. I would mention this already from the start and come back to its motivation at the end of the section.
• l.441-442, p.17: You praised the benefit of using a non-Gaussian likelihood (sum of Gaussians) in Sect. 3.2, so it is confusing to read about Gaussian composite likelihoods here. My eye cannot distinguish the likelihoods in Fig. 6 from Gaussian distributions (which also touches on the topic in a previous comment about \( \beta \) and \( \gamma \)), the former should be more heavy-tailed. I would just drop the "as Gaussian distributions".

• l.45-462, p.17: I found these couple of phrases (ending with "Fig. 6c.") of little value for the paper, as they essentially give a technical explanation of the resampling procedure. Or did I miss something?

• Fig. 6, p.18: You may want to point somewhere in the paper to the outlying GOZCARDS likelihood in panel (j) which has a clear impact on the 99\% credible region. I found this a nice illustration of the multi-modal joint likelihood.

• l.536-539, p.20: Is the transition prior of PF(SAGE) bootstrapped from the transitions of the two SAGE-composites rather than from the four composites?

• l.553-554, p.20: This phrase is strange, perhaps part of it is missing. How can local time of equator crossings be near-polar to attain near-global coverage?

• l.589, p.23: OSIRIS is a limb-viewing instrument, so should not be mentioned here.

• l.606, p.23 (and elsewhere): The notion of "trend" carries various meanings in the community. Personally, I preserve "trend" for any long-term component that can not be attributed to known atmospheric processes or to known measurement artefacts. I advocate the phrasing "drift" or "artificial trend" in the latter case, which is much less confusing than blending it in with actual geophysical signal.

• Sect. 4.3: How did you go from the time series in 10 degree latitude zones to regression results over 30 degree wider latitude belts? Average the time series, then regress? Please explain this briefly in the manuscript.

• l.752-754, p.28: Do you (or Laine et al) have an explanation for this instability? If you don’t, perhaps mention that this deserves further investigation. This feature is striking and should be better understood.

• Fig. A2, p.34: Specify the latitude range unless the Figure is for the entire data set at 1 hPa.

• l.894, p.34: Add units to "small drifts of 0.5\%". I know many people refer to 0.5\% per year (or 5\% per decade) as small, but they actually mean small compared to the stability of the data records. It is definitely not small compared to the actual trend being targeted, so this is a very unhappy phrasing in my opinion. Same comment for "[...] SAGE and HALOE agree to within 5\% in terms [...]", what is the unit?

• l.895, p.35: Hubert et al. (2016) is the first official report of a significant drift of 5\% per decade of HALOE relative to sonde and lidar. Previous studies are consistent with this negative drift, but the results were not significant. I suggest to nuance your statement slightly: "[...] Nazaryan and McCormick (2005) and Hubert et al. (2016) suggest that MOST datasets used in GOZCARDS have good stability.”

• Algorithm 1 (Step 3), p.36: See earlier comment, the composite likelihoods are not Gaussian according to Eq. 3.

• Algorithm 1 (Step 4), p.36: See earlier comment, isn’t this just a technical description of implementation? I would summarise this to one phrase.

• l.950, p.37: The word "original" is somewhat ambiguous here; it could mean the real, observed time series or the fit (with/without Gaussian noise?) to that time series. I find the phrasing "undamaged" time series better here (also used as label in Fig. A4b).
• l.962, p.38: I don’t see months 20-30 as a second exception, they are just a result of the offset of all four composites in month 50.

• l.973-974, p.39: This phrase confused me, do you mean that the vertical resolution of SBUV degrades at lower altitudes? Perhaps you wanted to say "This difference in vertical resolution becomes more important at lower altitudes."

3 Technical corrections

• l.125, p.4: The Penckwitt et al. paper was (and will likely) not (be) published. Please double-check this with G. Bodeker, one of the authors. Alternatively, Tummon et al. (2015) probably remains the best reference for this data set, as it has a concise summary of the merging method, satellite instruments and data versions.

• l.181-182, p.8: Not sure where the "this" refers to in ", this describes the updated version [...]."

• l.207, p.8: Reference to Fig. 2b, should be to Fig. 2c.

• Fig.3, p.9: It is hard to discern blue from black markers/lines in print. Perhaps this Figure will benefit from a deviation of the colour scheme used in the rest of the paper.

• l.233, p.10: Replace "SAGE-II-based instruments" by "SAGE-II".

• l.283-286, p.11: The section references are incorrect.

• l.378, p.14: Smaller values of $\beta$ encode more faith in individual observations rather than less, no?

• l.390, p.15: "compositeS".

• l.435, p.17: Remove "(Algorithm 1)" following "the preparation step".

• l.672, p.25: "deseasonAlised".

• l.730-731, p.27: A "negative decrease" is, strictly speaking, an increase. Could be replaced by "[...], and insignificant decreases at [...]".

• l.878, p.34: Remove duplicate "to" in "[...] tending to to cancel [...]".

• l.914, p.35: Add a reference to Algorithm 1 on the next page, so this section is not empty.

• l.937, p.36: Typo in "sectioN".

• Fig. A4, p.38: Fix the legend label for "DLM" in the bottom panel.

• Fig. A5, p.39: Fix labels in caption, should be (a) and (b) instead of (b) and (c).

• l.975, p.39: Add a space before reference to Bhartia et al.

• l.1168-1174, p.45: Update reference to AMT version of manuscript.