Interactive comment on “Copernicus atmospheric service for stratospheric ozone: validation and intercomparison of four near real-time analyses, 2009–2012” by K. Lefever et al.

Anonymous Referee #1
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The manuscript presents an overview and evaluation of near real time ozone products generated by four data assimilation systems under the auspices of MACC. Validation results of total ozone column and vertical structure (where available) comparisons against independent ground-based, sonde and satellite observations are given. A case study of the extreme Arctic ozone depletion in the spring of 2011 is discussed.

It is important for the scientific community interested in monitoring atmospheric composition that the performance and quality of these data sets be documented. Consequently, this work fits well into the ACP profile. I find some of the results very interesting. The manuscript is well organized and the set of comparisons is quite comprehensive.

Therefore I recommend this paper for publication. However, the presentation suffers from multiple shortcomings and, in my opinion, it requires some significant revisions before it becomes suitable for publication. By way of disclaimer, there are a lot of things that I like about this work but in this review I have to focus on the shortcomings.

General comments.

1. In my view, the main weakness of the study is in the interpretation of the results presented. The authors don’t explore the reasons behind the differences between the assimilation systems. If explanations are given they are often speculative (phrases like ‘this may be due to . . . ’ are used). For instance, BASCOE appears to have the best performance and IFS-MOZART is worse despite the fact that it assimilates more data. Why? Section 4.1 discusses alternating bias patterns in IFS-MOZART; Section 5.2 ascribes unstable performance of IFS-MOZART to assimilation of UV/VIS but offers no explanation as to why these observations would degrade the analysis. Section 6.2 demonstrates that turning off UV/VIS is beneficial but, again, it doesn’t explain why. At the face of it this is surprising because SBUV agrees quite well with MLS – if its averaging kernels are taken into account. Are they used in the assimilation systems? If not then one has to contend with large smoothing errors inherent in nadir data. In the case of SBUV it may help to interpret this in the context of [Kramarova et al., 2013]. I think that the interplay between different input data types is an important aspect of chemical data assimilation and this study is the right place to dive into these issues - but none of them gets much (if any) attention. Addressing this point can be considered a major revision of the manuscript.

2. This paper will be of interest to scientists less familiar with data assimilation. It is important to make it easy to read for someone who is not fluent in DA terminology. The word ‘model’ is used in several places where a better term would be ‘data assimilation system’. There are phrases like ‘models which assimilate data’ or (P12482) ‘. . . the model underestimates total ozone . . . ’ where you are really talking about analysis. Be more precise. Models don’t assimilate anything!
3. Explain the advantages of assimilating data as opposed to simply using retrieved observations. In particular, the conclusions section says that the four analyses perform well where data are present and not so well where there are no data. The reader may wonder why you need assimilation at all? Why not just use observational data?

4. Figures: The labels are too small to read without strong magnification. Almost all plots have that problem.

5. ‘Introduction’ and ‘Conclusions’: It would be good to state clearly why ozone analyses and forecasts are done. What is the scientific and/or policy-making related purpose of this undertaking?

Specific comments

Abstract. Too long. In particular, when you state a result you do not need to provide explanation. For example, on P12463 L20, everything after the comma can be deleted.
P12464 L1 ‘may be related’. That’s speculative. I would delete this part of the sentence.
P12465 L12 ‘information of satellite observations’ → information obtained from satellite observations.
P12468 L4. ‘(…) with a vertical resolution of about 3 km.’ Add ‘in the stratosphere’. It’s actually closer to 6 km in the mesosphere.

Section 2.1.3. Please clarify. Do SACADA and TM3DAM use both, total ozone and profiles from GOME-2? How many independent pieces of information do the profiles have?
P12469 L 23. ‘(…) of which four are currently still operational: NOAA-16/17/18/19’ Please, double check that. As far as I know NOAA-18 SBUV is not operational (http://www.oso.noaa.gov/poesstatus/spacecraftStatusSummary.asp?spacecraft=18) and NOAA-16 SBUV data are not usable at the moment.

Section 2.1.4. As for GOME-2, I suggest discussing the number of independent pieces of information and/or smoothing errors inherent in ozone partial columns retrieved from nadir observations. For SBUV there is a good analysis of smoothing errors in Kramarova et al., 2013. Typically, the actual information content in the vertical is much less than suggested by the number of layers. This applies to GOME-2 as well.

P12470 L6. The MLS Data Quality Document lists two components of error: precision and accuracy. Are both taken into account in these estimates – and in assimilation?
P12469 L24. Version 8 SBUV retrievals are given on 21 layers between 1000hPa – TOA. Does IFS-MOZART combine the layers somehow to get six? How is it done?
P12470 L6-10. Again, MLS errors are reported as precision and accuracy. Is the combined error 10%? When you say that most biases disappear in v3.4 you are talking about the accuracy component. Please, be more precise here.

P12472 L2. ‘The system also includes a parameterization of the effects of Polar Stratospheric Clouds (PSCs) on the gas-phase species’. This is vague. What kind of parameterization? Does it include catalytic ozone destruction? While Table 2 provides references to model chemistry schemes it would help if it were stated explicitly whether or not each of these models includes heterogeneous ozone loss on PCS (as is done in the case of IFS-MOZART). This is important because the paper talks about the representation of ozone holes in the analyses.
P12472 L14. ‘In contrast, IFS-MOZART assimilates other satellite instruments apart from Aura MLS, but those are measuring only ozone as species relevant for stratospheric chemistry.’ I don’t understand this sentence.
P12475, L13. ‘The background variance is set to 50 %.’ Please, state this more clearly: The background error variance is 50% of what? The units of variance are the square of the units of the field itself. You can’t get, say, ppmv2 by taking 50% of ppmv. The proportionality coefficient has to be a dimensioned factor.
P12476 L26. Define \( \mu \)
Looking at Figure 2, the two large positive excursions in SACADA are punctuated by sharp dips before the onset of the ozone hole. This likely indicates some underlying errors in the model chemistry. I think this warrants more discussion than what is provided in the following subsection, which basically simply explains that there are no data in the polar night.

\[\text{positive biased} \rightarrow \text{positively biased}\]

‘Latitudes not covered by observations can therefore only be influenced via tracer transport.’ – and chemistry.

Does this mean that only the two sonde measurements directly below and above a model level were used in the interpolation? Doing it this way will introduce a lot of noise. Assuming that assimilated ozone at a given layer represents the mean mixing ratio within that layer, the best strategy would be to integrate the portion of a sonde profile that falls within that layer and compare that (pressure weighted) integral with the mixing ratio value from assimilation. Looking at Figure 4, there is a lot of scatter in the sonde data vs. assimilation. I wonder if some of it is due to the way the data are interpolated. I suggest that the sonde – assimilation comparisons be repeated using mean (mixing ratio integrated w.r.t. pressure and divided by delta p) sonde observations within each layer.

‘Mixing ratios are appropriately scaled by an altitude independent factor using the model’s one ozone profile.’ I’m not sure if I understand. Do you mean that the background (guess) profile is scaled proportional to the ozone column increment by applying the transpose of the observation operator? People who are not well versed in data assimilation will wonder if this is some ad hoc trick or if it is part of the mathematics of the best linear unbiased estimation.

I wouldn’t say that the tropopause location is hard to define. We just go ahead and define it. The hard part is to correctly represent the sharp ozone gradients near the tropopause.

How do these standard deviations compare to the ACE-FTS errors?

‘Anticorrelation between levels’. Three levels are shown. Which two are anticorrelated? From the plot it looks like maybe 50 hPa and 100hPa but it’s not very clear. What is the correlation coefficient?

I don’t see how the missing MLS data can explain the differences between BASCOE and IFS-MOZART given that, as you say, the effect in March is minimal, there are no ACE data in all of April, and both systems were assimilating MLS for most of May. It’s more likely that the difference arises from either different chemistry schemes or the fact that IFS-MOZART assimilated UV/VIS data the whole time and BASCOE did not. Some of the UV data may have influenced the composition inside the vortex either directly or through transport. This harks back to my general comment (1).

‘(…) may be due to the fact…’ – very speculative. Does this mean that UV/VIS data degrade the analysis? Why is that? See my general comment (1)

Again, can you explain why UV/VIS degrade the performance?

Please re-write. You don’t have to go into details here but I don’t think it’s fair to say that ozone depleting gases are ‘trapped’ in PSCs. If anything is trapped it is nitric acid. The PSCs particles serve as a surface for heterogeneous reactions, which convert the reservoir species into ClO and Cl2. Then, in the presence of sunlight, active chlorine catalytically destroys ozone.

You mean underestimation of mixing ratio not ozone depletion, right? It’s clear from the plot but not from the context.

‘(…) may be related’: are there any other differences between the two runs of BASCOE? If there aren’t than the slightly better performance is due to different versions of MLS (not ‘may be’).

Either the extended range of MLS or the absence of other ozone data
is beneficial. This data withholding experiment alone is not enough to determine which.
P12495 L22-26. So what happens in the stratosphere in this additional experiment and
why? See my general comment (1).
P12498 L1. ‘(…) using the models one ozone profile’. I don’t understand this sentence.
You also had it in P12487 L5. Is some additional scaling used on top of assimilation of
total ozone? If so, please explain.
P12498 L18-27. I couldn’t agree more! We need follow-ons to MLS and MIPAS etc.
Just one point: For ozone we have OMPS – Limb Profiler on Suomi-NPP (or we will
have it as soon as the data are released) so we are not completely limited to UV/VIS
nadir data.
Technical Corrections:
P12468 L4. ‘0.02 hPa to 215 hPa’ → 215 hPa to 0.02 hPa. You have altitude from the
top to bottom so the pressure range should also go from the bottom to top.
P12476 L13. Drop the word ‘however’.
P12482 L20 positive biased → positively biased
Figure 3. The labels on the color bars are unreadable without magnification.
Figure 4. Again, please re-plot it using larger labels.
P12492 L17 spring → spring
P12498 L10. ‘require the assimilation’ → require assimilation
Reference
SBUV smoothing errors: an example using the Quasi-Biennial Oscillation

Atmos. Meas. Tech. Discuss., 6, 2721-2749, 2013
Interactive comment on Atmos. Chem. Phys. Discuss., 14, 12461, 2014.