

## ***Interactive comment on “The MACC reanalysis: an 8-yr data set of atmospheric composition” by A. Inness et al.***

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Please find below our replies to Referee 2.

General comments: Section 2.2: I suggest including equations that describe the data assimilation process (i.e. the cost function). This will be useful in the next section when the equations for the observation operator is presented. Retrieval diagnostics such as averaging kernels could do with some clarification. In particular I would point out that these come about due to the optimal estimation approach to retrieving data from the satellite measurements - this may also be helpful in explaining why the NO<sub>2</sub> observation operator is different later in the manuscript (I assume NO<sub>2</sub> isn't retrieved using optimal estimation).

- We have included the equation of the cost function and changed the text to: "ECMWF has used an incremental formulation of 4-dimensional variational data assimilation since 1997. In 4D-Var a cost function is minimized to combine the model background and the observations to obtain the best possible forecast by adjusting the initial conditions. In its incremental formulation (Courtier et al. \ 1994) 4D-Var can be written as ... where  $dx$  is the increment,  $B$  the background error covariance matrix,  $R$  the observation error covariance matrix (comprising of observational and representativeness errors), and  $H$  a linear approximation of the observation operator.  $d=y -Hxb$  is the innovation vector,  $y$  the observation vector and  $xb$  the background."

- We have added in section 2.2.1: "The averaging kernels come about due to the optimal estimation approach to retrieving data from the satellite measurements and indicate the sensitivity..."

Section 4: I think the manuscript would benefit from some general comments on how improvements could be made in a future reanalysis of this type. The appendix goes some way to describing some of the relevant issues, which are vitally important to potential users of the reanalysis product, but it strikes me that the authors could link this to similar future efforts in a couple of short statements. In light of some of the issues described throughout the manuscript, a statement in the conclusion on how these issues may affect the usability of the reanalysis as a research tool will be helpful to the reader. - We added these sentences at the end of the first paragraph of the conclusions: "These discontinuities limit the usability of the reanalysis as a research tool for assessing the state of the climate or studying interannual variability. The most important issues are summarized in Appendix A. A future reanalysis of atmospheric composition would benefit from using an improved CTM, or chemistry routines integrated in the IFS, better emissions, improved bias correction (e.g. ensure that bias correction is anchored properly and does not drift, more sophisticated bias correction for CO), and the exploration of more datasets, especially profile data if available."

Figures: Labelling of the figures is very minimal. Much of the information is included in

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the figure captions but I would prefer to see clearer labelling of the axes including units on the figures themselves. - After consultation with the editor we have decided to leave the figures as they are. We can change them if needed.

Specific comments: Page 31249, Line 7: please clarify that this is horizontal resolution - it may also be worth indicating the vertical resolution as the reanalysis spans the troposphere and stratosphere. - We have added "horizontal" so that the sentence now reads: "...at a horizontal resolution of about 80km for both the troposphere and the stratosphere."

Page 31250, Line 4: rearrange the sentence so that the definition is before the acronym. - Done

Page 31253, Line 3: OH has not been here although it is further down the paragraph - suggest moving to here. - Done

Page 31253, Line 11: in what respect is tropospheric ozone harmful? one or two references might be useful. - Changed the sentence to :"... and at high concentrations near the surface harmful to human health."

Page 31254, Line 19: has GRG been defined previously? - Weve moved the definition here from page 31255,114.

Page 31256, Line 5: what are the differences, if any, in the time resolutions between IFS and MOZART-3? some information of the dynamical and chemical timesteps would be useful for the reader. - Added:"The timestep is 1800s for the IFS and 900s for the CTM."

Page 31256, Line 12: suggest changing "had already" to "has been". - Done

Page 31258, Line 10: suggest using "photochemical" rather than "chemical". - Done

Page 31259, Line 9: it would be helpful to the reader if a formula for the data assimilation process could be referred to here. - A formula of the cost function has been added

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at the beginning of section 2.2 and a reference to this equation has been added here.

Page 31261, Line 25: while the averaging kernels have to be provided by the data producers I would point out that the averaging kernels come out of the optimal estimation approach to the retrieval. - Done.

Page 31262, paragraph starting at line 26: some of the terms in this paragraph read like technical jargon. I think it would helpful to the reader to explain what the bias correction is to begin with rather than assuming knowledge of the ECMWF system. I would understand that the bias correction is applied to retrievals of the same parameter from different instruments but this isn't particularly clear here. Also it isn't clear what the term 'anchor' refers to and the bias correction description may help with this.

- We have added some sentences to this paragraph and it now reads: "Retrievals of the same parameter from different satellite instruments can have biases with respect to each other or to the model. Assimilating biased data violates one of the underlying assumptions of data assimilation, namely that the data should be unbiased, and therefore a bias correction scheme has to be applied to the data. Without this, the assimilation would either have to be limited to one retrieval product for a reactive gas, or data would be used that are inconsistent with each other or with the reactive gases forecast. In the MACC reanalysis, the variational bias correction scheme ..."

We think the term anchor is already defined clearly in the current text: "...were used as anchor for the bias correction, i.e. no bias correction was applied to these data."

Page 31263, Line 26: suggest changing "within" to "throughout". - Done.

Page 31264, Line 18: the description of the GFED emissions should also make it clear how non-carbon species emitted by biomass burning are determined - i.e. I assume emissions factors are used, from which source?

- We have included the following sentences about the emission factors in section 2.4: "The emission factors for GFEDv3.0 are calculated using an update of the fire-type-

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dependent emission factors compiled by Andreae et al. (2001) and the actual values are listed in van der Werf et al. (2010). An analogous dependency on Andreae and Merlet (2001) holds for GFAS. Its actual emission factors are listed in Kaiser et al. (2012). In both cases the most significant update is the inclusion of emission factors for peat burning based on Christian et al. (2003). The NO<sub>x</sub> emission factor is expressed as the equivalent amount of NO. For savannah fires, its value has been revised downwards from 3.9 g(NO)/kg(dry matter) to 2.1 g(NO)/kg(dry matter). The NO<sub>x</sub>/CO emission ratios calculated for the different fire types from the emission factors used in GFEDv3.0 and GFAS range from 0.005 for peat fires in GFAS to 0.035 for savannah fires in both GFAS and GFED3."

Page 31269, Line 23: change "apart" to "apart from". - Done

Page 31270, Line 5-6: a lot of recent work has been done to better understand issues related to the model errors when assimilating CO data (e.g. Jiang et al., 2011). In particular the convection scheme used in the model transport can lead to quite large discrepancies which would also impact on the long-range transport as the authors state. It would be useful to the reader if the authors could make a stronger statement on this and put the MACC reanalysis in the context of other studies looking at this.

- We do not want to put too much emphasis on the long-range transport, because it is more a speculation and needs some more investigation to understand it properly. We have therefore removed the sentence referring to long range transport from the text.

Page 31270, Line 28: suggest replacing "only little" with "limited". - Done.

Page 31271, Line 8: I appreciate that relatively coarse model resolution would not capture fine-scale structure in the MOZAIC profiles, I would at least expect it to get the background CO mixing ratios right - a comment from the authors on this would be helpful.

- We think this is sufficiently discussed in the paragraph, because we mention potential

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problems with the emissions or a missing process in the CTM. Further studies are on the way to investigate this.

Page 31272, Line 11-12: there is also higher insolation over the equator - could this also help to explain the lower ozone columns? - We have changed the sentence to: "In the tropics, where there is slow large scale ascent and higher insolation..."

Page 31272, Line 15: please clarify that UV instruments can't measure anything (not just ozone) in the polar night because there is no backscattered solar radiation. - we have added: "...when the UV instruments GOME, SBUV/2, SCIAMACHY and OMI can not observe the ozone field because there is no backscattered solar radiation."

Page 31273, Line 1: are these Brewer-Dobson spectrometer observations? - Changed this to "Brewer and Dobson Spectrophotometers"

Sentence beginning on Page 31273, Line 29: I thought this would be fairly fundamental atmospheric science but it is poorly written here. I thought that net ozone production occurs in the tropical upper stratosphere and is transported poleward and downward by the meridional branches of the Brewer-Dobson circulation. The large-scale ascent in the tropics brings other chemical species into the stratosphere such halocarbons and N<sub>2</sub>O which can further influence stratospheric ozone photochemistry and it isn't clear to me if ozone is transported from the troposphere to the stratosphere as the authors state. I could be wrong but this should be clarified before publication (a reference could also be helpful). - We have shortened the paragraph so that it now reads: "The vertical structure of the MACC ozone field can be seen in the seasonal mean cross sections in Fig. 12. Ozone concentrations in the stratosphere are the result of the balance of ozone production, ozone loss and transport. The figure clearly depicts the ozone layer which is at higher altitude in the tropics than in the extratropics. The concentrations in the tropics are lowest in DJF when the upwelling branch of the Brewer-Dobson circulation is strongest. At the same time, the ozone layer in the NH extratropics is strongest because descent brings ozone rich air down. In SON, the impact of the chemical

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ozone destruction over Antarctica is clearly visible. Here the ozone layer is very thin and partial pressure values around the ozone maximum are less than 9 mPa in the seasonal mean.

Page 31276, Line 1-2: this isn't particularly clear from the figure. It will be helpful if the authors could quote some numbers to clarify how large is "large". -There was a problem with the colour scale of Fig. 15 and it didn't distinguish correctly between positive and negative values. We have change the colour scale of the figure so that it is clearer.

Page 31277, Line 2: is the model horizontal resolution the only issue that could contribute to this? could vertical transport also play a role as with the CO assimilation? As with the CO, I would expect the model to at least capture background ozone mixing ratios. - Changed the sentence to: "...that either the horizontal resolution is not high enough to reproduce the high values seen over polluted airports, that there could be problems with the vertical transport or that the differences are due to the chemical coupling..."

Page 31277, Line 23: include numbers to clarify what "small" means. - Done. It now reads: "The bias of the reanalysis is around 5% in the free troposphere in the NH extratropics, and small and negative (-10-5%) in the tropics."

Page 31277, Line 26: clarify the "good agreement" between the two datasets - from the figure the bias appears to be fairly persistent throughout most of the reanalysis period at + 20-30%. The subsequent sentences clarify the discrepancies but it only appears to be "good" at particular time periods. - With good agreement we mean agreement between the sondes and the MOZAIC data. We have changed the sentence to: "....shows similar biases for both data sets."

Page 31279, Line 20-23: could the differences also be due to no ozone observations being available at nighttime in the assimilation? does the sensitivity, information content and data availability change as a function of season in the assimilation? What about

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vertical mixing between the free troposphere and PBL? Previous studies (Parrington et al., 2009 and Foret et al., 2009) have looked at this and could be useful to cite here.

- Yes, all this is possible too and we have added these sentence to the text: "Other factors could be issues with the vertical mixing between the free troposphere and the boundary layer or the fact that fewer observations are assimilated during the night when no UV data are available. Parrington et. al (2009) and Foret et al. (2009) assessed the impact of assimilating ozone data on surface ozone concentrations, and further studies are necessary to determine the diurnal impact of the ozone assimilation on the surface ozone in the MACC system."

Sectio 3.2.4: it isn't clear if this section is all that necessary and distracts a little bit from the flow of the manuscript in describing the MACC reanalysis - isn't the perspective inherent to the comparison against independent observations? I would recommend removing this section prior to publication.

- We think that this subsection is important because it compares the quality of the ozone analysis with the well know ERA-Interim reanalysis and illustrates that despite some short comings the MACC ozone field is of better quality than the ERA-Interim ozone field. We would like to keep this subsection.

Page 31281, Line 3: change "as" to "such as". - Done

Page 31282, Line 3: the NO<sub>x</sub>/CO emission ratio should be described in the model set-up section as I pointed out above.

- This has now been include in section 2.4, see answer to question about p31264, line 18.

Page 31283, Line 6: what about large positive biases over Scandinavia in DJF/SON? I assume these are small relative biases? some numbers to quantify the magnitude of the biases would be helpful in the text.

- No, this is a large relative bias. We think it is related to a problem in life time that

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leads to too much transport into these areas. A sentence about this is included at the end of the paragraph. " Over Northern Europe the reanalysis is higher than the IUP-SCIAMACHY data in DJF and SON. This might be related to a problem in life time leading to too much transport of pollution into these areas."

Page 31284, Line 20-27: could this be related to data availability? the authors have already alluded to the challenges of assimilating a species like NO<sub>2</sub> with a short photochemical lifetime. does SCIAMACHY observe less in the winter?

- No, that is not a problem at these latitudes.

Section 3.4: is the section describing the HCHO analysis really necessary? after all this is a paper describing the MACC reanalysis and there are small differences between the control and reanalysis HCHO.

- We think it is useful to have this section, because it is helpful to give the user and idea of quality of the HCHO data in the same document as the other species. Even though no HCHO data are assimilated the data are available from the MACC data server and it is useful to document their quality and have them included in the paper so there is a published reference for them.

We have uploaded a revised version of the paper and of fig15.png.

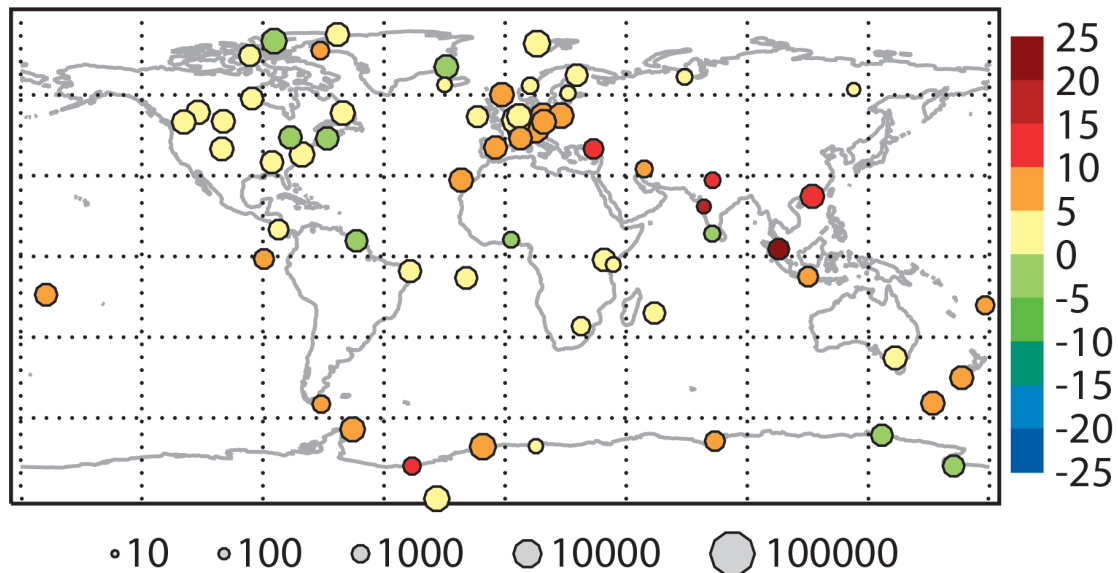
Please also note the supplement to this comment:

<http://www.atmos-chem-phys-discuss.net/12/C13524/2013/acpd-12-C13524-2013-supplement.pdf>

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**Fig. 1.** Revised Fig15. Caption unchanged from original version

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