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Atmospheric Chemistry and Physics Discussions

# *Interactive comment on* "Results from a new linear $O_3$ scheme with embedded heterogeneous chemistry compared with the parent full-chemistry 3-D CTM" *by* B. M. Monge-Sanz et al.

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**Response to A. Geer (Referee)**

We thank Alan Geer for his review. His comments are repeated below (*in italics*) and our responses are given in **bold text**.

*This paper introduces a linear ozone chemistry scheme with a consistent representation of heterogeneous chemistry. The new scheme is validated inside a CTM, and it is shown to work well in representing polar ozone loss, providing a better way to represent heterogeneous chemistry than that currently used in the ECMWF system. The*



*material is well presented and is ready for final publication with only minor changes.*

*1) p12995, l6 - To my knowledge, only O3 and H2O are prognostic variables in operational NWP systems. Include CH4 and CFCs in this list only if there are references to back this up (and please supply them).*

**We did not mean to imply that all the species mentioned are prognostic variables, however all of them are used in the radiation operators of the ECMWF data assimilation system (DAS), influencing therefore the initialisation of the NWP model forecasts. In the ECMWF DAS the Cariolle and Déqué scheme is used for stratospheric ozone (Cariolle and Déqué, 1986; Cariolle and Teyssèdre, 2007), an empirical parameterisation is used for stratospheric $H_2O$ (Dethof, 2003) and $CH_4$ and CFCs are represented only as climatologies at the moment.**

**We will edit the corresponding paragraph to make it clearer in the final ACP paper.**

*2) p12996, l25-29 - Any criticism of cold-tracer approach needs to be balanced and properly justified. As it stands, the paper says that the COPCAT approach is superior, but without including any new evidence. Ideally (though not required for publication) this paper would test it alongside the other approaches. Failing that, discussion of the cold tracer is necessary, but can only be speculative. The following points should be considered:*

**Providing a quantitative comparison between COPCAT and an alternative cold-tracer approach is not straightforward due to the implicit treatment of the heterogeneous chemistry in our scheme. Ideally, to do this we would have to calculate one version of COPCAT using only the gas-phase chemistry in the CTM, add the cold-tracer and then compare its performance to the COPCAT version containing all chemistry. However, when calculating the "gas-phase COPCAT", it would be difficult to establish which reactions to include and which ones to leave out, while still providing a parameterisation consistent with the current knowledge of**

**ozone chemistry.**

**For the ECMWF coefficients, a comparison between the default local temperature heterogeneous term and a cold-tracer is published in Cariolle and Teyssèdre (2007).**

*a) Yes, the cold-tracer may need retuning from year to year. But COPCAT does too, as stated later in the second to last paragraph of the introduction.*

**Our results have shown that for a 10-year simulation differences between the COPCAT scheme and the full-chemistry ozone field are small, using the same coefficients for all years. Differences with the full-chemistry model are similar in the early 1990s and early 2000s, indicating that the coefficients can safely be used for periods in which the chemistry conditions are relatively stable (e.g. chlorine loading). This shows a more robust approach in terms of adaptability than that of a cold-tracer, which needs retuning for dynamical variability and not just for variability in chemical conditions.**

*b) The cold-tracer would likely do a much better job in non-zonally symmetric situations, particularly the Arctic winter. A discussion does occur later in the introduction, but ideally all discussions on the cold-tracer should be merged.*

**The cold-tracer will always have the disadvantages of requiring annual tuning to accommodate to the particular meteorology and of following only temperature conditions. In principle, the way the heterogeneous chemistry is implicitly treated in COPCAT, would allow for realistic performance in non-zonally symmetric situations as well, by adding longitudinal variability to the coefficients calculation. This would make the scheme similar to the performance of a cold-tracer in terms of following zonal asymmetries, with the advantage of not only following low temperature air masses but also taking into account previous air processing. However, then the scheme would be more dependent on the particular meteorological conditions of the year used to compute the coefficients.**



**We will add this brief discussion and we will also rearrange the cold-tracer discussion in the final ACP paper.**

*c) A cold-tracer, by definition, requires an extra tracer, but in NWP, this extra computational overhead would generally be undesirable.*

**Yes, the cold-tracer requires one extra tracer to keep track of the low temperature air masses. And one of the advantages that CD-like schemes have for operational centres is that they require only one tracer to simulate ozone distributions. In fact, avoiding the inclusion of an additional tracer is the main reason why ECMWF has not implemented the cold-tracer available with the last version of their coefficients (Cariolle and Teyssèdre, 2007), as an alternative to the localised temperature term. We will add a couple of sentences on this in the final ACP manuscript.**

*3) p12999, l23 - Please introduce the TOMCAT box model and describe how it relates to SLIMCAT. NWP readers will not necessarily know what a box model is.*

**OK, we will do this in the final ACP paper.**

*4) p13000, l3 - "initial state" - what is this? From the previous sentence, a January-December 2000 mean is implied.*

**Here "initial state" refers to the SLIMCAT fields used to initialise the box model on the 15$^{th}$ of each month. We will rephrase this part to make it clear.**

*5) p13000, l12 - "initial state on 15th of each month" - what does this mean? "Initial state" implies some re-initialisation is going on. Is "state at 00Z on 15th of each month" intended?*

**Yes, we meant initial state of the box model runs, which are initialised using the fields from the 3D SLIMCAT run. We agree with the reviewer that it would be clearer to say the "SLIMCAT variable state on the 15$^{th}$ of each month". We will rephrase this.**

*6) p13000, l24 - "... ozone is initialised with the average field over the first day" - why is this done? What is the significance?*

**It was done to avoid the introduced perturbation to smear out, which would otherwise occur for regions with fast photochemistry.**

*7) p13002, l10 - ".. linear squares fit to the points..". If only two or three points are fitted, why use least squares? I'd have expected either two or three point numerical differentiation to be applied here. Please explain / justify your fitting in more detail in the text.*

**OK, we will do this for the final ACP paper.**

*8) p13003, 17 - Give a published reference to the HALOE data.*

**The most comprehensive validation study for HALOE ozone data is that of Brühl et al. (1996), which is already cited although later in that paragraph. Since that validation study, HALOE has gone through two major revisions. The HALOE version used in our study corresponds to the third public release (v19). The data were provided to us by William Randel and Fei Wu from NCAR (personal communication included in the manuscript). Comparison of these HALOE ozone data with SAGE II measurements was carried out in Morris et al. (2002) and McHugh et al. (2005) compared them against ACE observations.**

**We will edit the text to make all this clearer.**

*9) p13003, l21 - Please state the percentage of cases where the annual mean is substituted in place of the monthly mean.*

**We only use HALOE data when comparing with annually averaged results from the model runs, we have not substituted the monthly mean by the annual mean. We will clarify this in the final paper.**

*10) p13004, l4 - "differences can only be due to the use of COPCAT instead of the full*



*chemistry". What is the effect of any approximations in going from SLIMCAT to the box model, TOMCAT?*

**In that sentence we implied that in the 3D SLIMCAT simulations the only difference is the use of the linear ozone scheme or the full-chemistry approach, everything else (e.g. resolution, numerics, meteorology) is the same.**

**The COPCAT scheme has been implemented in SLIMCAT and compared to the full-chemistry ozone field from SLIMCAT. There is no box model involved when comparing the performance of the scheme and the full-chemistry. The box model is only used to calculate the coefficients, and there are no differences in the chemistry employed by the box model and the SLIMCAT configuration used to produce run323.**

**A different matter is whether the calculation of the scheme itself could be improved by, for instance, using higher resolution than that used in run323. A brief discussion on this is already in the Summary section, we will expand it in the final ACP paper.**

*11) p13004, l25 (and later discussion on p13008) - Could the 60DU bias in Arctic regions come from the use of zonal mean chemistry in COPCAT being inappropriate to the highly non-zonal nature of the northern stratospheric winter? This is one area where the cold tracer would be expected to do better. Please discuss in the text.*

**The fact that the COPCAT coefficients have been calculated from zonally averaged output from the 3D full-chemistry model, and were provided as altitude/latitude lookup tables neglects some longitudinal features. In particular features at the edge of the polar vortex will not be correctly simulated.**

**This is a general limitation common to all CD-like ozone schemes. A cold-tracer would be able to track such variability in a more realistic way, but still the need of an additional tracer and of frequent tuning of the parameters would need to**

**be overcome. Besides, the cold-tracer approach does not consider air activation taken place outside the low temperature region (see also response to comments above related to the cold-tracer).**

**Another factor affecting the bias in the Arctic region is the fact that coefficients are calculated for the 15$^{th}$ of each month. And coefficients on the 15$^{th}$ of March/September do not provide realistic loss rates for the sunlight levels found later in the month in the Arctic/Antarctic regions. This could easily be improved in future versions of the scheme by providing coefficients twice a month.**

**We will discuss all this in the final ACP paper.**

*12) Figure 6. The blue and black lines are indistinguishable.*

**This colour problem did not show in the article proofs we printed out, we will redo the figure using more clearly distinguishable colours to make sure it does not depend on the specific printer.**

*13) p13005, l12-23 - Discussion on mid and upper-stratosphere biases. Please cover the following in the paper: a) Why use the CHEM2D / Fortuin and Kelder climatology? What about the climatology in the ECMWF scheme, how does this compare? This would perhaps have been more relevant to the rest of the paper.*

**Our interest in testing an ozone reference term mainly based on observations was to evaluate effects of biases in the model-based ozone reference we use by default (reference term based on output from SLIMCAT run323). The reference term supplied with the ECMWF v2.9 coefficients comes from the 2D photochemical model MOBIDIC. Therefore, attribute differences between the COPCAT runs using the MOBIDIC-based $O_3$ reference term and the SLIMCAT-based $O_3$ term would not be possible, due to the number of differences between both CTMs.**

*b) Please state what observations the Fortuin Kelder climatology is based on.*

**Ozonesonde stations used in the FK98 climatology from the surface to 10 hPa**



**are described in Fortuin and Kelder (1998), together with Solar Backscatter UV (SBUV-SBUV/2) satellite observations used between 30-0.3 hPa. Also, additional scaling to total ozone mapping spectrometer (TOMS) measurements was performed.**

**We will include this information in the final ACP paper.**

*c) Please note the existence of much previous work on substituting one ozone climatology for another in a linear scheme, e.g. Eskes et al. (2003), McCormack et al. (2006), Geer et al. (2007), all of which are already in the reference list.*

**The FK98 climatology was used in Eskes et al. (2003), instead of the default term in the McLinden et al. (2000) parameterisation, to minimise conflicts within the data assimilation system (TM3DAM). However, no comparison between both ozone reference terms (default and FK98) was provided.**

**In McCormack et al. (2006) the FK98 climatology was used because it was the one used to initialize their model at upper levels, therefore, reducing additional biases. But they did not compare results using different climatologies either.**

**Geer et al. (2007) did show a comparison for the ECMWF v2.1 scheme using either the default supplied climatology term or the FK98 climatology. Their results suggested the existence of biases in the default climatology with respect to FK98.**

**We will develop this discussion in the final ACP paper.**

*d) Figure 7 - blue and black solid lines are indistinguishable ; HALOE (the red line) should be included in the key on the figure itself.*

**We will redo this figure using more clearly distinguishable colours.**
**We will also include the line for HALOE in the figure key.**

*e) "the minimum .. is around 60DU higher". The Fortuin and Kelder climatology does* *not have values for latitudes greater than 80 degrees. Could interpolation/extrapolation to 90S have caused the problem?*

**Yes, the ozone climatology we have used is the one provided with the CHEM2D scheme coefficients (McCormack et al., 2006). This means that the FK98 climatology was extrapolated outside the range where observations are available. In CHEM2D, at latitudes higher than 80 degrees the ozone value was extrapolated linearly in latitude based on the latitudinal ozone gradient defined by the two most poleward values (J. McCormack, personal communication). And this fact will most probably have an effect in the underestimation of the ozone loss at the highest latitude (90 degrees).**
**We will clarify this in the final paper.**

*14) p13006, l6 - "both schemes underestimate column values" - this could be linked back to Fig. 7*

**We will edit the text to show that the column underestimation agrees with the profiles in Fig. 7.**

*Typos etc.*

*1) Abstract, l15-16 Full stop after "observations"; capitalise "However"*

*2) p12995, l10 "by" -> "in" ; remove "numerical"*

*3) p12995, l14 "considered point" -> "point considered"*

*4) p12995, l24 "come from" -> "are derived from"*

*5) p12996, l2 "obtained with" -> "are derived from"*

*6) p12996, l24 "discussed in Sect. 1" - we are in section 1 already*

*7) p13002, l12 "shown ranges" -> ranges shown" ; "dependence with" -> "dependence on"*



**All these typos will be corrected in the final ACP paper.**

**References**

Dethof, A., Aspects of modelling and assimilation for the stratosphere at ECMWF, SPARC Newsletter, 21, 2003.

McHugh, M. et al., Comparison of atmospheric retrievals from ACE and HALOE, Geophys. Res. Lett., 32, L15S10, doi:10.1029/2005GL022403, 2005.

Morris, G. A. et al., A comparison of HALOE V19 with SAGE II V6.00 ozone observations using trajectory mapping, J. Geophys. Res., 107(D13), 4177, doi:10.1029/2001JD000847, 2002.

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