Re: Minor Revision of ACPD, Atmos. Chem. Phys. Discuss., 14, 5561-5609, 2014

Dear Dr. Jöckel,

thank you for your answer on our revised submission. We reconsidered the manuscript with respect to your comments:

> *"Unfortunately I think it is NOT sufficient that you answered the questions A, B, C, D of referee #2 in the discussion only. The essence of these answers needs also to be included in the revised manuscript, because it is important information and the revised manuscript must stand for its own at the end. The same holds for the requested "discussion about dynamic effects" in the conclusions. Here, it is not sufficient to just add additional references.*
>
> *Therefore, before final publication in ACP, please*
> *- add the essence of your answers to questions A,B,C,D at an appropriate position in the revised manuscript,*
> *- add a real discussion on the role of dynamic effects in the discussion / conclusion section."*

Adding the essence of answers A-D:

Thank you for reminding us of the problem which we inattentively omitted in our revised submission. We included the essence of our answers on questions A-D of referee #2. A brief recap of the questions is

A) "How do you infer the diurnal variation of a gas?"
B) "How do you take into account possible latitudinal variation in gas distribution?"
C) "Please explain how you separate transport and chemical effects."
D) "Have you done some kind of smoothing?"

In order to prepare the manuscript in a way that questions A-D do not arise while reading it we did the following changes to Sect. 2.2 (pages and lines refer to the latest version of our manuscript, the different color may help you to identify the paragraphs addressing the specific questions A-D):

5/131-150
This entire paragraph is revised and the essence of the answers A-D is included:
'In our configuration, the WACCM model produces four-dimensional fields of gases, dynamics and reaction rate coefficients with an output frequency of one hour. The entirety of these fields give a detailed view on conversion of specific chemical branches. For instance, a generic bimolecular reaction of species A *and* B *react to a product at the reaction rate R which is given by*

$$R = k\,(\mathrm{A})(\mathrm{B}) \qquad (1)$$

where k refers to the reaction rate coefficient and (X) *stands for the concentration of species* X*. The four-dimensional WACCM fields of k,* A *and* B *in combination with Eq.(1) yield the reaction rate R at any time and location within the limits of the model resolution. The spatio-temporal fluctuations of the reaction rate are governed by those of the atmospheric gas concentrations and the reaction rate coefficient.*

The four-dimensional hourly WACCM output of gases, dynamics and reaction rates is often transferred from universal time (UT) to local solar time meridian (LSTM) by

$$\mathrm{LSTM} = \mathrm{UT} + \varphi\ 24\ \mathrm{h}/360°, \qquad (2)$$

where φ refers to longitude in degree. The 5° longitudinal resolution of the WACCM simulation corresponds to a resolution of 20 minutes in LSTM. For consistency, the hourly WACCM output at each grid point is interpolated to a series with a temporal resolution of 20 minutes in UT. After the transformation to LSTM the 20 minutes temporal resolution is maintained for the analysis and the illustration in our figures. These resulting four-dimensional fields in LSTM allow to study also regional effects which is an advantage over diurnal variation sampled from different longitudes. In the following the term 'LT' is used as synonym for the inconvenient 'LSTM'.'

Dynamics discussion:

Referring to the missing discussion about dynamics we added in Sect. 5 a discussion about advection effects.

12/323-347
We discuss the polar region in winter where WACCM shows fluctuations which can not be explained by photochemistry.
'At the polar regions in winter Fig. 6 shows fluctuations in D_O3 which can not be explained by photochemistry. We relate these effects to advection at diurnal and shorter time scales which is supported by the strong gradients in the ozone field at the polar vortex. Technically, the continuity equation of ozone and other species is fully solved by the WACCM model. However, we question if WACCM can adequately simulate the effects since realistic advection at diurnal and shorter time scales requires an almost perfect representation of the main coupling processes of the atmospheric layers (e.g. two-day waves, sudden stratospheric warmings and gravity waves).
For instance, in the middle atmosphere vertically propagating gravity waves from below play a key role for dynamics. The gravity waves are excited when stable stratified air flows over orography, or by internal heating or shear (Garcia et al., 2008). These waves show a growing momentum flux with height and deposit heat or momentum to the background state while dissipating in the middle atmosphere. The WACCM model incorporates a gravity wave parametrisation solving for a spectrum of monochromatic waves and for those generated by flow over orography (Garcia et al., 2008). The parameters of the gravity waves are tuned to simulate basic climatological features as temperature and dynamics consistent with observations (Garcia et al., 2008). Richter et al.(2008) found that WACCM at a low spatial resolution of 4° latitude by 5°longitude shows less variability in the stratosphere than at higher model resolutions (e.g. gravity wave drag is about 25% enhanced). Although higher resolution increases variability it does not improve the representation of the mean wind and temperature in the stratosphere (Richter et al., 2008). We infer, that the 4°latitude by 5°longitude resolution is well tuned to generate good agreement to climatologies but it seems likely that gravity wave-induced advection processes on time scales of one day or less are underestimated in our free-running WACCM simulation. Here, we can state that the free-running WACCM simulation shows weak signatures of diurnal ozone variations at the polar vortex which are possibly caused by short-term, periodic advection processes in combination with strong, spatial ozone gradients. Further investigations with a nudged model or reanalysis data are planned.'

In the conclusions we removed a single sentence and added a new paragraph about this topic.

18/564
Removed sentence:
'On the other hand the WACCM model might underestimate dynamical effects near the polar winter vortices where effects based on photochemistry are weak and transport might play a major role.'

18/571-581
Included discussion about dynamics:
'In the polar region in winter our simulation showed diurnal ozone variation which we related to advection at diurnal and shorter time scales. We suggest that these advection processes at the polar vortex and the associated diurnal ozone variations might be stronger in the real atmosphere since the low resolution, free-running WACCM simulation underestimates the influence of gravity waves on middle atmospheric dynamics (Richter et al.,2008). Therefore, a realistic representation of middle atmospheric advection at shorter time scales seems to overstress the prospects of the free-running WACCM model. Sato et al.(2009) showed that high resolution modelling at 60 km horizontal and 300 m vertical resolution internally generates realistic propagation and momentum deposition of gravity waves without any gravity wave parametrisation. Further research on advection in the polar region in winter could base on data from such high resolution modelling or from data assimilation systems with well reflected dynamics at diurnal and shorter time scales.'

The end of this paragraph holds implications for future research and suits well to our preliminary study which picks up these ideas and is planed to be submitted soon. Further, we changed Eq. 9 in Sect. 3 to be the continuity equation including advection.

7/187-194
Eq. 9 is changed to be the continuity equation and the related text is assimilated to these changes:
'Chemical and photochemical reactions are handled by the chemistry module of WACCM which bases on the MOZART model. The WACCM model solves the continuity equation of ozone which describes photochemistry and advection by

[*Here Eq. 9 is changed to be the continuity equation including advection...]*

where φ is the ozone flux. The reactions involving NO, NO2, H, OH, HO2, Cl and Br are parts of catalytic ozone depletion cycles which are limited by the rates of intermediate steps (Johnston and Podolske, 1978).'

Before discussing Fig. 1 in Sect. 4 we included a sentence which relates the conversion rates to the terms of the continuity equation (this relates also to question C of referee #2).

7/206
We added a sentence to better understand the chemical branches with the help of Eq.(9).
'The following conversion rates relate to the photochemical sink and source terms of Eq.(9).'

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Further changes:

Aside your comments we found some minor points which we changed in the manuscript. The changes are listed point-by-point:

4/108-109
We found that the the reference of the MOZART model is wrong or more precise it does not address the correct version. We changed the reference and the sentence on the MOZART model.
'The chemistry module of WACCM bases on the Model of Ozone and Related Chemical Tracers (MOZART, Kinnison et al.,2007).'

4/117
We corrected 'Version' to 'version'.

5/154+159
At the definition of D_O3 and T_O3 'day' is replaced by 'from 00:00 to 24:00 LT'.

17/545
Replacement of 'from' by 'with'.

19/585
Double 'can be' is deleted.

Appendix
Corrected typo: 'missing'

Thanks again for your efforts and critics which considerably improved the manuscript.

Best regards
Ansgar Schanz