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Atmospheric
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Interactive comment on "Parameterization of middle atmospheric water vapor photochemistry for high-altitude NWP and data assimilation" *by* J. P. McCormack et al.

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General comments

Compared with the existing standard for the parameterization of middle atmospheric water vapor photochemistry in NWP models (ECMWF, 2006), this work introduces much-needed latitudinal and seasonal dependences. Unfortunately in its present state, the paper reads more like a progress report than a completed scientific study.

In short, one can not exclude that the apparent success of the parameterization (better agreement between forecasts and analyses) is due to the inclusion of the same analyses in the reference state of the parameterization as those used to validate the

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forecasts. This is a serious issue, for which I see no other solution than the replacement of the reference state used in the recommended set-up (EXP2) by an average of the analyses obtained *before* the forecast dates. This is of course a requirement to allow future real-time applications.

I think that publication in ACP requires a more complete description of the system, one major addition (comparison of forecasts with independent observations) and one major revision, i.e. the use of a reference state averaged from analyses *preceding* the starting date of the forecasts. More details are given below.

Specific comments

The CHEM2D-H2O parameterization is developed in a classical and consistent manner. It basically consists in prescribing a reference state for the distribution of water vapor, and the relaxation times towards this reference state. Since photochemical tendencies are considered as perturbations from the reference state, the relaxation times represent here the time scales for water vapor photochemistry as computed by the CHEM2D model. They are given as a function of latitude, pressure and season which is an improvement compared with the one-dimensional approach of the ECMWF parameterization.

The choice of the reference state for the distribution of water vapor is by far the biggest difficulty in this study. In theory, it should correspond to the mixing ratio at photochemical equilibrium as computed by CHEM2D. In practice, it is obtained from observations in order to avoid large biases between the modeled and assimilated constituent values. This approximation has become standard in the development of linearized parameterizations of ozone photochemistry, which often use monthly zonal mean climatologies.

The same approach is attempted here for water vapor but systematically fails to deliver forecasts closer to the corresponding analyses than those using the ECMWF parameterization. The authors propose to use instead, as reference state for their parameterization, a monthly average of all analyses for the month and year used in the study

(June 2007). This set-up allows them to obtain smaller biases (between analyses and forecasts) than the set-ups based on a climatological reference state or on the ECMWF parameterization. But it is based on a reference state that includes analyses (hence observations) *posterior* to the initial times of the forecasts. Since the validation of the parameterization is limited to a comparison between these forecasts and the *same* analyses, this set-up prevents any conclusive validation of the parameterization.

In my view, the use of averaged analyses rather than a published climatology limits the applicability of the CHEM2D-H2O parameterization to NWP and data assimilation, excluding unconstrained long-duration simulations. This limitation is acceptable but should be discussed in the text.

The study suffers from several other important shortcomings:

- The failure of the parameterization based on a UARS climatology (EXP1) could be partly due to inadequate photochemistry in CHEM2D and/or inadequate transport in NOGAPS-ALPHA. But this is impossible to assess because the two models are not adequately described with respect to some processes important in the mesosphere/lower thermosphere region (see especially points 2 and 6 below).

- No details are given of the assimilation set-up: what are the assimilation scheme, error statistics and observation operators used here? The latter point is especially important in view of the very low vertical resolution of the Aura MLS observations in the upper mesosphere. Is this low vertical resolution taken into account in the assimilation system, and how is this done if it is the case? In the absence of any discussion about background, representativeness and observation errors, a fundamental question remains open: are the observations and analyses closer to the truth than the forecasts?

- This doubt would be alleviated by a comparison of the forecasts with independent (non-assimilated) observations, which is a requirement for any proper validation of a NWP/DA system. No such comparison is done here: the forecasts are only compared with the corresponding analyses.

I have some further specific comments:

1) Figure 1b lists three channels for the photodissociation products of H_2O. Sander et al (2003), the only reference given for the photochemical scheme of CHEM2D, lists only the H+OH channel. Brasseur and Solomon (2005, 3rd edition) mention the H_2+O(1D) channel, which could be significant in the mesosphere. But I do not know any reference for a channel producing 2H+O. What are the exact references used for these three channels, and what quantum yields were used ?

2) The radiative transfer and absorption of solar UV radiation, as modelled in CHEM2D, is not described. The modelling of this process was not described either in McCormack et al (2006). But this point is especially important because as stated p. 14003, "H_2O photolysis is an important effect for medium-range forecasts in this region" [above 0.01 hPa]. Hence the following questions must also be adressed in section 2:
- How is parameterized the absorption of solar UV radiation by molecular oxygen in the Schumann-Runge bands ? and at Lyman-alpha ?
- The absorption cross-sections of methane and water vapor at Lyman-alpha are not specified by Sander et al (2003). What are the values used by CHEM2D ?

3) Figure 3 shows a net production of water vapor in the winter hemisphere, near 80 km poleward of 50° latitude. This enhancement is attributed to production by OH + HO_2. Is this based on specific model output or is it an hypothesis ?

The possibility of an enhanced production but OH + HO_2 is justified by "poleward transport of OH from the tropics to higher latitudes where OH becomes very long-lived in the upper mesosphere (Brasseur and Solomon, 1986)". OH here must be replaced by HO_x, as OH itself never becomes long-lived enough to be directly influenced by transport. Furthermore, at 80 km the HO_x lifetime shown by Brasseur and Solomon (2005) barely becomes comparable with the time constants of the (residual) zonal and meridional winds - so it is not clear that HO_x can be transported from the tropics to the higher latitudes. Finally, Brasseur and Solomon (2005) do not mention the season and latitude used to calculate these lifetimes. If this explanation holds, it should be supported by specific model output, e.g. latitude-pressure plots of the HOx lifetime and vertical profiles of the H2O productions by each relevant reaction. Note that such plots would be of great value by themselves.

4) Page 14007, line 9: the assimilation system is described in detail by Eckermann et al. (2008, submitted to JASTP) but this paper is not yet published. Hence the present paper should deliver some basic information about the assimilation scheme used by NOGAPS-ALPHA.

5) Section 3.1: what about the dehydration due to PSC sedimentation ? Does the NOGAPS-ALPHA model take into account this process ? PSC sedimentation has a very large impact on water vapor above the Antarctic in springtime, between 30 and 100 hPa. If PSC sedimentation is not taken into account, this must be stated clearly as it implies that the modelled water vapor is not useful in the lower stratospheric polar regions. If PSC sedimentation is included, this should be mentioned in the paper with proper references.

6) The CHEM2D and NOGAPS-ALPHA models seem to neglect molecular diffusion, while the importance of this process in the upper mesosphere has been demonstrated using a 2D model similar to CHEM2D (Chabrillat et al., 2002). Molecular diffusion could partly explain the underestimation of water vapor by NOGAPS-ALPHA in the mesosphere (figure 9), especially in view of the fact that this underestimation extends down to the stratopause in the polar winter vortex. Indeed, molecular diffusion results in an upward flux of water vapor in the homopause region while the polar winter mesosphere experiences a descent of air masses from higher levels. When molecular diffusion is taken into account, one would expect these air masses to be less dry than forecasted by the model.

7) End of section 3 (top of page 14011): "Solar UV fluxes in the CHEM2D model were set to solar minimum levels to match June 2007 conditions". This statement should be

moved to the description of CHEM2D (section 2). It would still be interesting to have the reference used for the solar spectrum shortwave of 200 nm, and especially to state what solar irradiance was used for the solar Lyman-alpha line.

Technical corrections

1) I was not able to print any figure past figure 4, even though I tried on 3 printers (using Postscript and HP drivers) from 2 different computers (Windows and Linux). This issue should be checked carefully.

2) Page 14013, lines 22–24 erroneously repeat the end of the previous sentence.

3) Page 14007: the references to Eckermann et al. (2008) appear as a footnote of the previous page. I propose to add "hereafter referred to as E2008" after the first citation and to use this label afterwards.

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