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Atmospheric
Chemistry
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Discussions

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

J. P. McCormack et al.

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We appreciate the referee's detailed review of the manuscript. We wish to emphasize that the main purpose of the paper is to describe the new CHEM2D-H2O parameterization. To this end, the paper is devoted to (1) providing a detailed description of the photochemical calculations comprising the parameterization and (2) demonstrating the sensitivity of the parameterization's performance to the assumed background (reference) state water vapor distribution. A complete evaluation of the NOGAPS-ALPHA middle atmospheric water vapor assimilation, which would involve detailed comparisons with independent observations, is not yet possible since the analysis system has not been run over sufficiently long periods of time. This will soon be rectified and we anticipate carrying out such a study in the near future. Based on the referee's com-

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ments, there are some shortcomings in the descriptions of the photochemical model and our methodology that we will address in our revisions.

The referee cites four main deficiencies in the manuscript. These consist of (1) the use of June 2007 zonal mean NOGAPS-ALPHA H_2O analyses to specify the background state in experiment 2 (EXP2); (2) Inadequate description of the the CHEM2D and NOGAPS-ALPHA models; (3) Insufficient detail in the description of the assimilation setup and reference to an unpublished manuscript; and (4) Lack of comparison with independent measurements. We address each of these issues below.

Issue 1: We agree that using the June 2007 NAVDAS H_2O fields to specify the background state in EXP2 is not an ideal choice, nor would it be a plausible approach for operational applications. Previous experience with linearized ozone photochemistry parameterizations (e.g., McCormack et al., 2006; Coy et al., 2007) showed that an analysis-based climatology is preferable in these types of simulations. Our choice for background reference state in EXP2 was motivated primarily by the fact that suitable middle atmospheric H_2O analyses at our disposal were limited to the June 2007 time period. To address the referee's concerns, we have performed an additional set of simulations, designated EXP4, using a background reference state based on zonal monthly mean H_2O mixing ratios from Aura MLS level 2 data for the months of June 2005-2008. This approach might be more consistent with possible operational applications and provides a more objective basis for comparison of the different H_2O photochemistry parameterizations. As we will show in the revised manuscript, the overall result remains the same: using an up-to-date observationally-based reference state with a latitude and seasonally varying photochemistry scheme yields the smallest overall values of A-F for the June 2007 period.

Issue 2: CHEM2D photochemistry has been used extensively in numerous studies of the stratosphere, mesosphere, and lower thermosphere. Earlier CHEM2D modeling papers cited in the manuscript (e.g., McCormack et al., 2006, McCormack et al., 2007, and references therein) have described in detail the method for computing radiative heating and photolysis by solar UV. We felt it was not necessary to duplicate these discussions, but we understand the referee's concern for adequate description of the relevant processes in the manuscript. Our revisions will address this concern. See also our response to specific comment 2 below.

Issue 3: The manuscript references a recent article by Hoppel et al. (2008) at the beginning of section 3.1 This article provides a complete description of the data assimilation setup, including the error statistics and observation operators. In response to the reviewer's concerns, we will provide a brief summary of the assimilation system's salient features in our revised manuscript.

The H_2O analyses used here does not account for the poor vertical resolution of the MLS measurements in the mesosphere. The full-width half-maximum of the MLS measurements is $\sim$4 km below the 1 hPa level, but increases to $\sim$12 km above the 0.1 hPa level (Lambert et al., 2007). Instead, a 2 km FWHM Gaussian averaging kernel is used in the assimilation. Although this is not the ideal setup, we preferred to constrain the analysis to the low resolution MLS profiles rather than allow the possibility that the assimilation could introduce spurious vertical structure in the H_2O fields.

For the analyses used here, the background error variance for water vapor in the upper atmosphere was set large enough to ensure that the analysis was highly constrained to the observations, producing a zonal mean distribution that is nearly identical to the MLS data. Our goal is to describe the H_2O photochemistry parameterization and evaluate its performance with a series of model hindcasts, not to validate the assimilation system. First steps in that effort have been undertaken elsewhere (Hoppel et al., 2008; Eckermann et al., 2008) and these efforts continue presently. As we show, once the parameterization is "tuned" so that the reference state reasonably approximates the observationally-based estimate of the true zonal mean H_2O distribution, it works quite well.

Issue 4: Comparison of our forecasts with independent measurements is problematic since, other than MLS, we do not know of any other global middle atmospheric H_2O data sets available for the June 2007 period. There are occultation measurements, e.g., ACE and SOFIE, but they are quite limited in spatial and temporal coverage. Eckermann et al. (2008) have undertaken a preliminary comparison of NOGAPS-ALPHA analyzed H_2O with SOFIE H_2O profiles (see their Figure 6, which is available at http://uap-www.nrl.navy.mil/uap/7646/publications/2008/Eckermann_aim_fig6.png). Based on this comparison, the analyses can be considered an accurate representation of the “true” water vapor distribution in the upper stratosphere and mesosphere and thus are of sufficient quality for use in the present study.

Replies to specific comments:

1) Table 4-1 of Sander et al. (2003), item B2, lists the $\mathrm{H + OH}$ channel, as the referee states. Their note for item B2 (pages 4-10 and 4-11) mentions that "at shorter wavelengths H_2 and O are also formed as primary products", i.e., the additional reactions listed in our Figure 1b. Sander et al. cite the study of Stief et al. (1975), which gives a complete listing of the H_2O photolysis channels. The channels 1, 2, and 3 in our Figure 1b coincide with channels D, C, and F of Stief et al. (1975). Stief et al. report quantum yields of 0.89 and 0.11 for the $\mathrm{H + OH}$ and $\mathrm{H_2 + O(^1D)}$ channels (channels 1 and 2 in Figure 1b), stating that additional channels (among them their channel F, the $\mathrm{2H + O(^3P)}$ channel) "are not expected to be significant" for the production of $\mathrm{O(^3P)}$. A more recent study by Harich et al. (2000) puts the quantum yields for the $\mathrm{H + OH}$ and the $\mathrm{2H + O}$ channels at 0.79 and 0.21, respectively, with no mention of the $\mathrm{H_2 + O(^1D)}$ channel. We have chosen yields of 0.78, 0.10, and 0.12 for channels 1-3 in Fig 1b, based on a synthesis of the available laboratory measurements.

2) For a description of shortwave radiative heating in CHEM2D, we refer to McCormack et al. (2006). In Section 2.2 of McCormack et al (2006), it is stated that CHEM2D computes the solar UV heating above 40 km explicitly using the same spectral distribution of solar UV and absorption cross sections as the photolysis calculations (details of which can be found in Summers et al., 1997, and references therein). The O_2 absorp-

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tion in the SR bands is based on the parameterization of Minschwaner et al. (1993). H_2O absorption is treated as in Siskind et al. (1994). O_2 and H_2O absorption at Lyman-α is based on the method of Lewis et al. (1983). CH_4 absorption at Lyman-α is not considered. We will add this discussion and the relevant references to our revised manuscript.

3) We have plotted H_2O production from various reactions in the CHEM2D model at 68S in June (see http://uap-www.nrl.navy.mil/uap/7646/publications/2008/nrl_chem2d_h2op.png). H_2O production by $OH+HO_2$ peaks near 0.01 hPa. This is due to a highly localized peak in model OH concentration at this level, which is in agreement with recent observations (see, e.g., Fig. 3 of Pickett et al., 2006). The referee is correct that HO_x, not OH, is being transported poleward. We apologize for the misstatement. We will clarify this explanation in the revision as follows: "This enhancement is due to poleward transport of odd hydrogen from lower sunlit latitudes into polar night where odd hydrogen becomes very long-lived in the upper mesosphere". We feel that further discussion of the details of HO_x chemistry in polar night is beyond the scope of this paper.

4) It was our hope that this article would be published by now, but that has been delayed. The most recent version of this manuscript can be viewed online at lttp://uap-www.nrl.navy.mil/uap/7646/publications/2008/Eckermann_aim_revised.pdf.

5) Presently, CHEM2D-OPP does not account for PSC-related sedimentation and dehydration. Water vapor in the lower stratospheric polar regions will be useful to the extent that the assimilated MLS H_2O measurements capture the effects of the dehydration over the course of the winter season. As stated in the manuscript, our primary focus is to provide accurate simulations of the background temperature and humidity conditions supporting formation of PMC's. These conditions will be fed into detailed microphysical models, so for now CHEM2D-H2O covers gas-phase photochemistry only. We will clarify this point in the revised manuscript.

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6) The reviewer is correct that neither model contains a treatment of molecular diffusion, which could affect our results at very high latitudes. However, based on the study of molecular diffusion of CO_2 by Chabrillat (2002), we would expect that the effects of molecular diffusion for H_2O would be relatively small given its lower molecular weight and lesser role in the radiative balance compared to CO_2.

7) We will move this to Section 2. Solar cycle variations in the solar flux between 1200 – 8000 Å are specified based on the measurements of Lean et al. (1997). The irradiance at Ly-α for solar minimum was 3×10^{11} photons cm^{-1} s^{-1}.

Technical corrections:

1) We were unaware of any difficulties printing the manuscript. The production staff may be able to help with this issue.

2) Corrected.

3) The footnotes were inserted by the ACPD production staff. We will consult with them to make this change in the revised manuscript.

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