Technical note: A stratospheric climatology for O₃, H₂O and CH₄ derived from HALOE measurements

J.-U. Grooß¹ and J. M. Russell III²

¹Institut für Chemie und Dynamik der Geosphäre I: Stratosphäre (ICG I), Forschungszentrum Jülich, Jülich, Germany
²Hampton University, Hampton VA, USA

Received: 11 April 2005 – Accepted: 15 April 2005 – Published: 12 May 2005
Correspondence to: J.-U. Grooß (j.-u.grooss@fz-juelich.de)

© 2005 Author(s). This work is licensed under a Creative Commons License.
Abstract

The Halogen Occultation Experiment (HALOE) on board the Upper Atmosphere research satellite (UARS) has observed mixing ratios of important trace species in the stratosphere over more than a decade since 1991. Here we present a climatology for the stratosphere compiled from the HALOE data for ozone, H$_2$O and CH$_4$ for the period from 1991 to 2002. In this approach, the data are averaged over equivalent latitude instead of latitude in order to correctly reproduce the gradients at the transport barriers like the polar vortex edge. The climatology is compiled for 5 degree equivalent latitude bins. The seasonal dependence is taken into account by choosing intervals of one month. The climatology is available as an electronic supplement.

1. Introduction

Global atmospheric models such as Global Circulation Models (GCMs) and Chemistry Transport Models (CTMs) need information about the spatial distribution of the chemical composition for some key tracer species, e.g. ozone or water vapor in order to achieve realistic results especially for the simulation of radiation. Both, the calculation of photo-dissociation rates of chemical species and the calculation of diabatic heating rates are needed to achieve realistic changes in chemical composition and to achieve realistic vertical transport, respectively. There are two different approaches to how the distribution of chemical species is used for these calculations. Either the information about the key chemical species is prescribed and stems from a climatology compiled from different data sets or it is derived from other models. These simulations are often called “off line” simulations. The second approach is to use the models own simulated values of the key species in the radiation code taking into account the feedback between chemistry and radiation. These simulations are often called “coupled” simulations. Both approaches, off-line and coupled, depend on a realistic compilation of a climatology from observations in order to validate the distribution of the key species on
which the radiation simulations is based. Here we present a climatology based on the satellite observations of the Halogen Occultations Experiment (HALOE) on board the Upper Atmosphere Research Satellite, that has taken measurements of stratospheric trace species since it was tuned on in orbit on 11 October 1991 up until today (Russell et al., 1993). The measured trace gases are ozone, CH$_4$, H$_2$O, HCl, HF, NO, and NO$_2$. Here we concentrate on ozone, CH$_4$, and H$_2$O observations. The HALOE instrument was validated against a variety of correlative measurements. The typical accuracy of the HALOE observations in the lower stratosphere is about 5% for ozone (Brühl et al., 1996), 10% for waver vapor (Harries et al., 1996) and less than 15% for CH$_4$ (Park et al., 1996). The vertical resolution of the data is between 2 km (O$_3$, H$_2$O) and 4 km (CH$_4$). The HALOE instrument uses the solar occultation technique and observes daily up to 15 sunrise and 15 sunset profiles of these measured trace species at about constant latitudes for both groups.

In the polar winters of both hemispheres, large differences of mixing ratios of chemical tracers inside and outside the polar vortices are a typical feature as well as large gradients at the vortex edge. HALOE does not sample the polar vortex on a regular basis. However, often the polar vortices are displaced from a circumpolar symmetry and large fractions of the polar vortex reach latitudes at which HALOE does observe. These air masses contain information from the polar vortex and typically have high potential vorticity (PV) values. Therefore the PV information was used when compiling the climatology presented here. The observations were sorted and combined with respect to equivalent latitude (Lary et al., 1995). The equivalent latitude was derived from PV using the analyses provided by the United Kingdom Meteorological Office (UKMO).

Figure 1 shows the latitude versus the time of year of the observations covered by the HALOE instrument between 1991 and 2002. Due to the solar occultation geometry, no observations are made during polar night and during continuous sunlight in high latitude summer. Figure 2 shows the HALOE coverage with respect to equivalent latitude. Clearly, the range of equivalent latitudes covered by HALOE is larger than the range of latitudes, especially during polar winter in both hemispheres. The covered period of
about 11 years corresponds to one period of the solar cycle. We do not include the most recent data since September 2002, since in 2002 there was a very unusual major warming in the Antarctic (Newman and Nash, 2005) and also the observations were less frequent after 2002.

There are other available climatologies used in GCMs and CTMs. E.g. Fortuin and Kelder (1998) compiled an ozone climatology for the period 1980–1991 from ozone sonde and satellite data. The main difference is that during that time the Antarctic ozone hole was not yet fully developed. Randel et al. (1998) also combined H\textsubscript{2}O and CH\textsubscript{4} measurements from HALOE with other UARS experiments (MLS, CLAES) to build a climatology with an equivalent latitude mapping from the observation of the period November 1991 to March 1997. Previous, more abbreviated climatologies of stratospheric water vapor have been published by Remsberg et al. (1990) and Russell and Swider (1991).

The presented climatology is used already in simulations. In the 3-D version of the Chemical Lagrangian Model of the Stratosphere (CLaMS) it has been used to calculate the diabatic heating rates that introduce vertical motion across the isentropic levels (Konopka et al., 2004, 2005). It was also used as input for the radiative transfer calculation from which the chemical photolysis frequencies are determined (Groß et al., 2002; Groß et al., 2004). A previous version of this climatology compiled from 6 years of HALOE data, 2-month averages and latitude bins instead of equivalent latitude is used in the ECHAM-5 model (C. Brühl, personal communication, 2004).

2. Method

The exact determination of the potential vorticity of a HALOE observation (required to determine equivalent latitude) was performed in the following way. First the observation location was transformed to a time on which UKMO analysis were available, i.e. to 12 h UT of the day of observation. This was done by (backward or forward) trajectory calculations from the time of observation until 12 h UT of the day of observation for
potential temperatures between 400 K and 2000 K using the CLaMS trajectory module (McKenna et al., 2002) and wind data from UKMO analyses. The equivalent latitude was then calculated from the PV on the respective potential temperature level for the so determined synoptic location.

Between October 1991 and August 2002, a total of 78,600 HALOE profiles of ozone, CH$_4$ and H$_2$O mixing ratio were then combined into bins of 5 degree equivalent latitude for 22 pressure levels between 316 and 0.1 hPa and 12 months. Each data point was assigned a weight equal to the inverse of its given accuracy. In doing this, data with low accuracy (e.g. at the bottom of some measured profiles or due to high aerosol content) only have a low contribution to the determined climatological average value. Since the area of the first and last equivalent latitude bin ($\pm 87.5^\circ$) is rather small and thus does contain not many data points, these bins were combined with the next bins at $\pm 82.5^\circ$.

The HALOE data points that have a reported retrieved accuracy of more than 2 times their mixing ratio are rejected from this compilation. Also data points that show unexpected large mixing ratios, more than 15 ppm ozone and more than 2.0 ppm CH$_4$ have been rejected. Further, it was requested that at least 5 HALOE observations were needed in a bin.

Since HALOE does not observe air masses during polar night, there are gaps in the data sets, even when using equivalent latitude mapping. To achieve a complete global dataset with the best estimate of the annual dependence, these gaps were filled. Typically, the air within the polar vortex is isolated from mid-latitudes and is diabatically descending over the time of the polar night. This causes e.g. the CH$_4$ mixing ratios in a given height to decrease with time. Thus, the latitudinal gradient increases through the polar nights. Therefore an extrapolation in latitude may not lead to realistic mixing ratios. In this study, we interpolated in time between the observations at the formation and at the end of the polar vortex at high equivalent latitudes, which should yield more realistic mixing ratios. In the following figures, the regions of these filled data gaps are shaded grey.

The advantage of this approach is that the climatology is compiled from a single data
source, therefore no biases between different sources have to be taken into account. This method is also possible because of the longterm stability of the HALOE observations. The experiment has been especially stable over the 13 plus years of operations thus far. The absolute change in signal level when viewing the sun outside the atmosphere has been no more than 0.5% in the H$_2$O channel and less than 2–3% in the CH$_4$ and O$_3$ channels. Even so, since the measurement is made by ratioing the signals obtained while viewing through the atmosphere to the signals measured outside the atmosphere, any change in the absolute signal level is removed. Also, other parameters such as spectral filter stability and field of view (FOV) mismatch effects have been carefully examined and no significant drifts in the instrument have been found.

The limit of this approach is, that data must be interpolated through periods of no observations, e.g. the polar night. Also species with a significant diurnal variation (e.g. ozone in the mesosphere) cannot be covered as the data always correspond to local sun rise or sun set. HALOE does not measure trace species in the troposphere regularly. Therefore this approach of compiling a climatology is best suited for the altitude range of the stratosphere.

3. Results

Figures 3 to 5 show examples if the compiled climatology for the ozone, H$_2$O, and CH$_4$, respectively. Shown are the months January, April, July, and October between 330 and 0.33 hPa. The other months are not shown here.

The ozone data displayed in Fig. 3 show a maximum of ozone mixing ratios of about 10 ppm in the tropics at 10 hPa. Also visible is the ozone depletion in the Antarctic vortex in October below 30 hPa, the so-called ozone hole, that was already well established during the period 1991–2002. Figure 6 shows the standard deviation (1σ) of the ozone mixing ratio of each bin. It is typically 5–15% in the mid to upper stratosphere and larger below about 50 hPa. Large variability of over 1 ppm is seen at the polar vortex edge in the southern hemisphere in October at the equivalent latitude of 65° S.
This is mainly caused by the variability of the size of the polar vortex and is also seen in the variability of CH$_4$ (not shown here).

Figure 4 clearly shows the increase of H$_2$O mixing ratio with increasing altitude throughout the stratosphere, that is caused by the CH$_4$ oxidation. Also, the strong dehydration in the Antarctic vortex in winter and spring is well pronounced in October. The increase of H$_2$O with decreasing altitude at the tropical tropopause may be underestimated, as for large tropospheric H$_2$O mixing ratios no precise HALOE observations are made since the lines employed for the HALOE H$_2$O retrieval are likely to be optically saturated.

The importance of CH$_4$ for radiation is smaller than ozone and H$_2$O. The major CH$_4$ sources are emissions at the earth surface and the major sink is its oxidation in the stratosphere. Due to its long lifetime, it is a good dynamical tracer and may be used to verify the simulations of meridional transport and the diabatic descent in the polar vortices. In the CH$_4$ climatology (Fig. 5), especially the diabatic descent over the winter in the polar vortices is clearly visible for both hemispheres yielding low CH$_4$ mixing ratios inside the vortex compared to mid-latitudes. The corresponding tracer gradient at the vortex edge is also clearly visible.

If this climatology is used for model predictions, the long-term trends of the considered species may be important. For the period considered here, the ozone hole was already well established. Towards the end of the period, the maximum expected mixing ratio of total inorganic chlorine (Cl$_y$) in the stratosphere was reached. The stratospheric Cl$_y$ mixing ratio, the precursor of ozone depletion, is expected to decrease slowly over the next decades, therefore the ozone mixing ratio averaged over the chosen period should be representative for the next decades in this respect. Water vapor in the stratosphere has been reported to increase. Rosenlof (2002) suggested 0.45%/year over last 45 years. A water vapor increase was also reported for the first 5 years of HALOE observations (Randel et al., 1999). However, it has been reported not to continue over the following years (Randel et al., 2004). This behavior can partly be explained by the increase of stratospheric CH$_4$ oxidation, caused by various factors such as the in-
crease of Cl$_y$ until about 1995 and the 11-year solar cycle (Röckmann et al., 2004). It is not clear whether this water vapor increase will continue in the future. Therefore, the presented H$_2$O climatology should be a good choice for the use in model predictions until 2015.

4. Online access

The compiled climatologies for ozone, H$_2$O and CH$_4$ can be obtained in the supplement as a NetCDF\(^1\) file (supplement acpd-2005-0129-sp0.nc, http://www.copernicus.org/EGU/acp/acpd/5/2973/acpd-5-2973-sp.zip) and as ASCII tables (ozone: supplement acpd-2005-0129-sp1.dat, H$_2$O: supplement acpd-2005-0129-sp2.dat, CH$_4$: supplement acpd-2005-0129-sp3.dat, http://www.copernicus.org/EGU/acp/acpd/5/2973/acpd-5-2973-sp.zip). The NetCDF supplement contains both the average data for each bin (equivalent latitude, pressure, month) and its standard deviation. Also, the number of observations corresponding to one bin is included. For data interpolated in time the number is set to $-1$.

5. Conclusions

The HALOE climatology presented here was compiled especially as input for GCM and CTM simulations representing the current status of the atmosphere. It uses a single stable data source and therefore avoids problems with biases between data sets. Despite some limitations discussed above, the climatology may be well suited as input for model simulations for the 1990s and for predictions until about 2015.

Acknowledgements. The authors gratefully acknowledge the United Kingdom Meteorological Office (UKMO) for providing the meteorological analyses, the HALOE team for providing a high quality dataset, R. Müller for fruitful discussions, and P. Bittihn for programming support.

\(^{1}\)For details of this file format see http://www.unidata.ucar.edu/packages/netcdf

2980
References


McKenna, D. S., Konopka, P., Grooß, J.-U., Günther, G., Müller, R., Spang, R., Offermann, D.,
Fig. 1. Coverage of the HALOE instrument. Shown is the latitude of the HALOE observation as function of time of year for all years indicated by different colors. Sun rise observations are depicted by thick lines and sun set observation by thin lines.
Fig. 2. As Fig. 1, but for equivalent latitude that was derived from UKMO PV on the 475 K potential temperature level. Sun rise observations are depicted by diamond symbols and sun set observation by crosses.
Fig. 3. Climatology for ozone for the months March, June, September and December. Light grey shaded areas indicate data interpolated in time.
Fig. 4. As Fig. 3, but climatology for H$_2$O.
Fig. 5. As Fig. 3, but climatology for CH$_4$.
Fig. 6. Standard deviation (1σ) in ppm of the climatology for ozone (Fig. 3) for the months March, June, September and December. Light grey shaded areas indicate data interpolated in time.