Atmos. Chem. Phys. Discuss., 3, 2261–2284, 2003
www.atmos-chem-phys.org/acpd/3/2261/

Atmospheric Chemistry and Physics Discussions

The impact of model grid zooming on tracer transport in the 1999/2000 Arctic polar vortex

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Received: 27 January 2003 – Accepted: 11 March 2003 – Published: 9 May 2003

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The impact of model grid zooming on tracer transport
M. M. P. van den Broek et al.

Abstract

We have used a 3D chemistry transport model to evaluate the transport of HF and CH_4 in the stratosphere during the Arctic winter of 1999/2000. Several model experiments were carried out with the use of a zoom algorithm to investigate the effect of different horizontal resolutions. Balloon-borne and satellite-borne observations of HF and CH_4 were used to test the model. In addition, air mass descent rates within the polar vortex were calculated and compared to observations.

Outside the vortex the model results agree well with the observations, but inside the vortex the model underestimates the observed vertical gradient in HF and CH_4, even when the highest available resolution ($1^\circ \times 1^\circ$) is applied. The calculated diabatic descent rates agree with observations above potential temperature levels of 450 K. These model results suggest that too strong mixing through the vortex edge could be a plausible cause for the model discrepancies, associated with the calculated mass fluxes, although other reasons are also discussed.

Based on our model experiments we conclude that a global $6^\circ \times 9^\circ$ resolution is too coarse to represent the polar vortex, whereas the higher resolutions, $3^\circ \times 2^\circ$ and $1^\circ \times 1^\circ$, yield similar results, even with a $6^\circ \times 9^\circ$ resolution in the tropical region.

1. Introduction

Both 2D and 3D Chemistry Transport Models (CTMs) are widely used to evaluate the understanding of atmospheric processes and to study how possible future changes in emissions will affect the composition and state of the atmosphere. One important focus of stratospheric research with CTMs is the depletion of ozone, notably in the polar vortex and at mid-latitudes. Both transport and chemical processes influence the ozone concentration, while its variability is mainly determined by dynamics (Chipperfield and Jones, 1999). To model stratospheric ozone and to estimate chemical ozone loss, it is therefore of great importance that ozone transport is modeled realistically.

ACPD

3, 2261–2284, 2003

Several studies tested modeled transport and investigated the related key model properties. In a 2-D latitude-longitude study on ozone depletion, Edouard et al. (1996) found a large impact of increasing horizontal resolution. Searle et al. (1998) repeated this study with contradictory results. Since both these studies concentrate on ozone depletion, both chemistry and transport are expected to influence this result.

One method to evaluate model transport separately is by simulating long-lived tracers, which can then be tested against observations. HF, for example, is such a tracer, which is used in this study. In an earlier model evaluation, Chipperfield et al. (1997) also simulated HF. They found a good agreement with observations, except in polar air where HF columns were underestimated. Rind et al., (1999) used CFC-11 and SF_6 to evaluate model transport across the tropopause and found no improvement when they increased the vertical resolution of their general circulation model (GCM). They suggested that dynamical properties such as wave drag and top altitude of the model should be improved with priority. Mahowald et al. (2002) point out that the choice of the vertical coordinate system, based on pressure or isentropes, impacts tracers such as water vapor and the age of air in the tropical stratosphere, with the isentropic coordinate system giving less diffusive and more realistic model results. A recent model intercomparison showed that the calculated age of air was too low in almost all models (Hall et al., 1999). It was also mentioned that within the polar vortex diabatic descent is underestimated in many CTMs and GCMs. However, more recent analysis showed that the descent rates inside the polar vortex in the 3D CTMs SLIMCAT and REPROBUS agreed reasonably well with observations (Greenblatt et al., 2002). Plumb et al. (2002) modeled transport of N_2O in the polar vortex for the same winter using the CTM MATCH. They found that N_2O was overestimated in the lower stratospheric vortex and suggested that cross-vortex boundary transport was not accurately calculated or that inner-vortex mixing was too intense. It was suggested that this was related to the underlying meteorological data, since doubling their original horizontal resolution of $2.8^\circ \times 2.8^\circ$ did not make a difference.

In this study we explore the effect of horizontal resolution on tracer distributions in

ACPD
3, 2261–2284, 2003

more detail by model simulations of HF and CH_4 during the 1999/2000 winter, focusing on the Arctic polar vortex. We also evaluate diabatic descent rates to interpret the calculated tracer distributions. We employ the newly developed chemistry transport model TM5 (Krol et al., 2003) to simulate HF and CH_4. TM5 contains a 2-way nesting zooming algorithm (Krol et al., 2001), which is employed here to study the effect of resolution changes on transport. HF and CH_4 are long-lived in the stratosphere and have lifetimes over 1 year below 10 hPa, and are therefore solely influenced by transport on shorter timescales. HF is produced in the upper stratosphere by photochemical breakdown of CFCs. It has no chemical sinks in the stratosphere and its only known loss mechanism is downward transport and subsequent wet deposition in the troposphere. CH_4 has the inverse profile, with higher values in the troposphere due to emissions at the earth surface from biogenic and anthropogenic activity. Concentrations drop with increasing altitude due to chemical loss by photo-dissociation and reaction with OH, O^1D and Cl in the stratosphere and reaction with OH in the troposphere. An important reason to focus on the 1999/2000 winter is the availability of observations of HF and CH_4 from the combined SOLVE (Sage III Ozone Loss and Validation Experiment) and THESEO (THird European Stratospheric Experiment on Ozone) campaigns.

Furthermore, a distinct polar vortex formed in the lower stratosphere after 1 December (Manney and Sabutis, 2000), which provides a good test case to study the isolation of the vortex.

We investigate modeled tracer distributions employing three different horizontal resolutions in the northern hemisphere, ranging from 9° longitude by 6° latitude to 1° longitude by 1° latitude. Van Aalst et al. (2003) carried out a model study with the same experimental set-up, using the MA-ECHAM climate model with assimilated meteorological data of the same time period.

The model experiments and the observations used are described in Sect. 2. Section 3 presents the model results and compares with the observations. Discussion and conclusions follow in Sect. 4.

ACPD

3, 2261–2284, 2003

2. Model experiments

2.1. Model description

We have used the new global three-dimensional transport model, version 5 (TM5). The model is an extended version of the TM3 model that has been used in several previous stratospheric studies (Van den Broek et al., 2000; Bregman et al., 2000; Bregman et al., 2001). The new model is able to zoom horizontally over a certain area, e.g. Europe or the polar vortex, by selectively increasing the horizontal resolution. Krol et al. (2001) explain the mass conserving two-way nesting algorithm and show first model results for tropospheric 222Rn. Figure 1 gives an impression of the zooming options in TM5 used in this study. Meteorological input for the model is provided by six-hourly ECMWF (European Center for Medium range Weather Forecasting) forecast fields of temperature, surface pressure, wind and humidity. The data extend up to 0.2 hPa. The method to calculate mass fluxes from ECMWF winds has recently been improved (Bregman et al., 2002). We used a 33-layer subset of the 60 layer fields that are taken into account in the ECMWF model, with a reduced number of levels in the tropospheric boundary layer and above 70 hPa. Before 12 October 1999 the ECMWF model used 50 vertical layers from which we derived a subset of 30 layers. Near the surface the model levels are defined as terrain following sigma coordinates whereas the layers above 100 hPa are defined at pressure surfaces. A hybrid of the two is used between the lower levels and the stratosphere. An example of the vertical grid in TM5, assuming a surface pressure of 1000 hPa, is shown in Fig. 2 together with the original ECMWF grid.

A mass flux advection scheme, using first order slopes (Russell and Lerner, 1981), is used to calculate tracer transport. A dynamical time step of 1800 s is applied for the coarsest grid (6° latitude by 9° longitude). For the 1° by 1° resolution a time step of 225 s is employed. Over the poles, the grid is reduced to avoid numerical instability through violation of the Courant Friedrichs-Lewy (CFL) condition (see Fig. 1). The physical parameterization of boundary layer diffusion and convection are identical to those of

ACPD

3, 2261–2284, 2003

The impact of model grid zooming on tracer transport

M. M. P. van den Broek et al.

the TM3 model (Peters et al., 2002), For instance, convection is calculated with the Tiedtke (1989) mass flux parameterization for cumulus clouds, including entrainment and detrainment in updrafts and downdrafts.

2.2. Experimental set-up

In this study, HF, and CH_4 are simulated during the winter of 1999–2000. Four zooming options have been investigated (see Table 1), with a horizontal model resolution ranging from 9° longitude by 6° latitude globally, up to 1° by 1° from 30° to 90° N.

The model integrations start at 1 September 1999. Initialization is based on zonally averaged observations of August and September 1999, obtained from the HALOE (HALogen Occultation Experiment) instrument aboard UARS (Upper Atmospheric Research Satellite) (Russell et al., 1993). In regions for which observations are not available (at the poles, in the troposphere and in a gap in the HALOE data between 43° N and 62° N), the initial concentrations are linearly inter- or extrapolated from nearby latitudes and/or altitudes. Removal of HF by wet deposition has been implemented in TM5 by assuming a lifetime of 5 days below 400 hPa, as in Chipperfield et al. (1997). The CH_4, concentrations in the lowest model layer are fixed at 1.76 ppmv. In the top two levels CH_4 and HF are constrained with HALOE observations (Randel et al., 1998), since chemical production (of HF) and destruction (of CH_4) are not included in the model. Sensitivity runs carried out by Van Aalst et al. (2003) show that stratospheric washout of HF and prescribing the top boundary concentrations for both tracers have only a small or negligible effect on the tracer fields for the integration period considered in this study. In addition, they found that ignoring chemical destruction of CH_4 causes a small deviation of less than 10%, and only above 20 hPa.

2.3. Observations during the 1999–2000 winter

The lower stratosphere was extremely cold during the Arctic winter of 1999–2000, especially in the early winter. Despite these low temperatures, the lower stratospheric

ACPD
3, 2261–2284, 2003

M. M. P. van den Broek et al.

vortex was weak until December and formed slowly compared to other cold winters. In the upper and middle stratosphere, a distinct vortex was already discernable on November 1st. By the end of December, the vortex was established throughout the stratosphere (Manney and Sabutis, 2000).

Several measurements of CH_4 and HF were used for comparison with the model results. (i) The balloon-borne Tunable Diode Laser Absorption Spectrometer (TDLAS) measured in-situ profiles of CH_4. The flights took place on 28 January, 9, 13 and 27 February, and 25 March 2000 and samples were taken inside, outside and at the edge of the vortex (Garcelon et al., 2002). (ii) Balloon-borne observations of HF and CH_4 were carried out with the JPL MkIV interferometer (Toon et al., 1999) in the inner vortex; both at the start of vortex formation on 3 December 1999 and close to vortex break up on 15 March 2000. (iii) The HALOE instrument observed both CH_4 and HF, collecting 8–15 profiles each day at two latitude bands (Russell et al., 1993). Usually, HALOE observations do not extend poleward far enough to reach the vortex, but on 20 February 2000 at 56° N some profiles were obtained at the edge of the vortex.

All these observations have been compared with the TM5 results. In addition, diabatic descent rates within the vortex, calculated by the model, have been compared with those derived from CH_4 observations (Greenblatt et al., 2002).

3. Results

3.1. Non-vortex HALOE HF profiles

Figure 3 shows a comparison of the model runs with HALOE HF profiles before vortex formation and of extra-vortex air while the vortex was present. The first three comparisons show profiles taken at 55° N, 48° N and 45° N, on 26 October, 5 December and 2 January, respectively. Apart from the coarse model run (GL_96), which overestimates HF between 20 and 2 hPa on 5 December 1999, modeled HF closely resembles the HALOE observations. In the later comparisons, on 20 February, 18 March and 30 April, the model results start to deviate from the observations, with HF being underestimated at all model resolutions at altitudes above 10 hPa. The maximum difference between model and observations occurs at an altitude of approximately 2 hPa, from 0.3 ppbv on 20 February to 0.5 ppbv on 30 April. Since this discrepancy only occurs in late winter at high altitudes, and the breakdown of the polar vortex took place mid-March (Manney and Sabutis, 2000), it can be speculated that the discrepancies may not be addressed to air originating from mid-latitudes, but from the polar vortex. Another explanation may be the fact that chemical production of HF is omitted in the TM5 model. However, as mentioned earlier, sensitivity studies including chemical production rates of HF show that this assumption can well be made during a stratospheric winter (van Aalst et al., 2003).

The GL_96 run generally yields somewhat higher values of HF compared to results from the three highest resolutions. It is interesting that these latter three experiments show very similar results in all comparisons. Note that the results from the GL96_NH32 run show no differences with the GL_32 results. This implies that for the integration period considered the representation of the tropics with a $6^\circ \times 9^\circ$ or $2^\circ \times 3^\circ$ resolution does not make a difference to the mid-latitude profiles.

3.2. TDLAS CH_4 observations in/out of the vortex

As a next step, we compare modeled CH_4 profiles to CH_4 profiles that have been measured by means of the balloon-borne TDLAS spectrometer, both inside and outside the polar vortex. The result is shown in Fig. 4. The estimated error for the observations is about 10%. Clearly, as in Fig. 3, the model results compare reasonably well with the observations outside the vortex, whereas the model results within and at the inner edge of the vortex indicate significant overestimation. It is remarkable that the model results are very similar for all zooming experiments, including 1° by 1° resolution. The Gl_96 run shows the largest overestimation, implying that this resolution is too coarse for a realistic representation of the tracer distribution.

The good agreement between model and observations outside the vortex was also

ACPD

3, 2261–2284, 2003

Title Page
Abstract | Introduction
Conclusions | References
Tables | Figures
◀◀ | ▶▶
◀ | ▶
Back | Close
Full Screen / Esc
Print Version
Interactive Discussion

indicated by the HALOE profile comparisons, especially below 10 hPa (see Fig. 3). However, inside and at the edge of the vortex the CH_4 vertical gradient increases with time, which is obviously not fully captured by the model.

3.3. MkIV inner vortex observations in early and late winter

In Fig. 5 TM5 results are compared to HF and CH_4 measurements by the MkIV interferometer. The observations were carried out inside the polar vortex in the beginning of winter, on 3 December, when the vortex was just formed in the lower stratosphere, and on 15 March 2000, just before the vortex break-up. Also in this comparison, HF is consistently underestimated and CH_4 is overestimated, both at the beginning and at the end of winter, and the differences between the model runs are similar to the earlier comparisons. However, on 3 December, the difference between model and observation occurs only above 50 hPa while by 15 March, the difference is seen throughout the lower stratosphere. Above 15 hPa HF steeply decreases and CH_4 increases on 15 March. PV maps indicate that the MkIV observations above 15 hPa were at the edge of, or outside, the vortex, which explains the gradient reversal.

3.4. HALOE HF longitude cross section

To examine the model performance on a larger scale, fifteen HALOE HF sunrise profiles, observed on 20 February 2002 at 56° N, have been compiled in a longitudinal graph and are compared with TM5 results (Fig. 6). The HALOE observations comprise both vortex and non-vortex air. For example, the feature with increased HF values between 90° E and 60° E and 50 hPa and 10 hPa represents air from the vortex edge. An increased vertical gradient in HF is visible below this area, between 100 hPa and 20 hPa. Another small feature of increased HF is discernable near 100 hPa, around 150° E–180° E.

More obvious than in the previously discussed profile comparisons, the Gl_96 run is too coarse to simulate transport within or across the edge of the vortex, since none of the observed longitudinal features is captured (Fig. 6b). All other model runs capture the observed longitudinal features well and again they produce similar results. On the other hand, the model underestimates the vertical gradient, especially inside the vortex between 150° E and 180° E. This is in agreement with the profile comparisons discussed above. The vortex air sampled at 56° N was situated at the edge, which can be seen from the modeled latitudinal cross-sections at 50° N and 62° N (not shown here). Excessive mixing may be a problem of the model there, due to the large gradients of HF across the edge of the vortex. At 62° N for example, situated more inside the vortex, the sharp vertical gradient matches much better with the HALOE observations at 56° N (see also van Aalst et al., 2003).

3.5. Descent rates

One likely cause of the model-observations discrepancies could be the underestimate of the diabatic descent by the model. We therefore evaluated the modeled vertical descent inside the vortex from 1 December to 1 April 2000, by comparing modeled with observed descent rates (i.e. derived from observations). The decrease of potential temperature along five CH_4 isopleths throughout the winter is shown in Fig. 7. The black lines shows inner vortex descent calculated from five observed profiles of CH_4 during the SOLVE/THESEO campaign (Greenblatt et al., 2002). The descent rates calculated from these CH_4 observations coincide with calculations carried out with a large number of inner vortex N_2O observations. The red lines represent the descent of CH_4 calculated with TM5. On each first day of the month, zonal winds and PV gradients were used to calculate vortex average profiles of potential temperature and CH_4 (see also van Aalst et al., 2003). We restricted the sampling to those profiles that were located within the vortex at all altitudes. The ECMWF PV fields have been used for this selection.

Figure 7 shows that, except for the "GI_96" run, the calculated descent rates during the winter agree quite well with those observed, except below θ ~450 K. The discrepancy increases closer to the vortex lower boundary, i.e. ~400 K, especially in early

ACPD
3, 2261–2284, 2003

M. M. P. van den Broek et al.

winter. Largest descent takes places from December to January, slowing down in February and being close to zero after the first of March. Increasing the horizontal resolution in the zooming experiments, either in the tropics or in the polar region, has no effect on these results.

Initially, modeled potential temperature on December 1 1999 has been synchronized with the observed θ profiles. Note that at the start of this calculation on 1 December, the offset in potential temperature for comparable CH_4 volume mixing ratios is about 50 K above 500 K. Around 450 K the offset is 20 K, whereas the offset has disappeared around 400 K and layers below. Thus, the model does not simulate the tracer fields above 450 K correctly, at the start of this comparison on 1 December. This is in agreement with the modeled overestimation of CH_4 and underestimation of HF with respect to the MkIV observations on 3 December, illustrated in Fig. 5. Similar pre-winter offsets are also found with the 3-D CTMs REPROBUS and SLIMCAT using the same set of observations (Greenblatt et al., 2002). Greenblatt et al. (2002) compared modeled and observed descent rates in a similar way as discussed here. Both models showed similar descent rates as TM5, although REPROBUS descent is somewhat faster than the observed descent in the beginning of winter in the lower stratosphere. In addition, similar results are found with the MA-ECHAM model (van Aalst et al., 2003).

4. Discussion and conclusions

During the winter of 1999/2000, the TM5 model is well able to simulate the HF and CH_4 distribution outside the vortex. Only later in winter and above 10 hPa TM5 overestimates the HALOE HF profiles outside the vortex. Even the coarsest resolution ($9^\circ \times 6^\circ$) provides reasonable results, although some dynamical features are not captured (for example, the upper stratospheric minimum in the CH_4 profile on 3 December 1999). Inside the vortex however, an overestimation of HF and subsequent underestimation of CH_4 is found for each resolution. The combined time series of the calculated and observed CH_4 and HF profiles (Figs. 4 and 5) show that the discrepancy arises mainly

ACPD

3, 2261–2284, 2003

during early winter (note that the discrepancy is already present on 3 December). Since the offset on December 3 is present in all experiments, including the highest resolution run (1° × 1°), it cannot be attributed to excessive mixing due to coarse horizontal resolution. It can also be ruled out that the discrepancies are caused by uncertainties in the experimental set-up such as boundary conditions at the top and at the bottom of the model and tropospheric rain-out, as was investigated by van Aalst et al. (2003).

Examination of the modeled diabatic descent rates reveals good agreement above a potential temperature level of 450 K throughout the winter. However, below 450 K, which is close to the bottom boundary of the vortex, the model underestimates the observed descent rates, but this underestimate only occurs before January. In contrast to the other model experiments, the calculated descent rates with the coarse resolution of 9° × 6° in the early winter are clearly wrong at all altitudes until the end of January.

Combining these results, we can conclude that although TM5 properly simulates the outer vortex, the model does not simulate the inner vortex observations well, especially during early winter. This may indicate that diabatic descent is not well represented in the model, thus the underlying meteorology from ECMWF does not properly represent the downward transport in the polar vortex. However, since the modeled descent rates agree well with observations at the corresponding θ-levels, the discrepancies in the other inner-vortex comparisons with observations may be explained by excessive mixing in the model. Possible solutions to reduce excessive mixing are for example increasing the horizontal resolution or using an isentropic coordinate system (Mahowald et al., 2002). In this study we increased the horizontal resolution of TM5 up to 1° × 1° for a relatively large area (northward of 30° N). Nevertheless, the discrepancies remain, which may be an indication that the accuracy of the vertical mass fluxes as provided by ECMWF is insufficient. In fact, Plumb et al. (2002) drew a similar conclusion, using different input mass fluxes. We need to point out that the impact of the vertical resolution has not been discussed. From recent model experiments we found that increasing vertical resolution did not change calculated ozone profiles significantly in the lower stratosphere (Bregman et al., 2001). Since the vertical gradient of ozone profiles is much larger than that of HF and CH_4, we expect a small effect of an increase of the vertical resolution. Nevertheless, it should be explored by performing model integrations with all (60) ECWMF layers, which we have planned for the future.

Another reason for the model discrepancies could be found in the vortex formation. The ECWMF extends only to 0.2 hPa where observations become sparse. Since the vortex was already formed on 1 November in the upper stratosphere (Manney and Sabutis, 2000), this region is very critical when simulating the early winter vortex. The descent rates are underestimated in early winter. This could be related to the neglect of ozone depletion in the model in regions where temperature profiles have not been measured and thus the ECMWF model runs freely without assimilated observations.

In our model experiments, the coarsest resolution of 6° latitude by 9° longitude produces relatively large errors. Especially in longitudinal variation as compared to the HALOE HF observations, and inner vortex descent are simulated unrealistically with this resolution. Such discrepancies should be considered when performing climate model integrations with similar resolutions (e.g. Pawson et al., 2000).

Finally, the applicability of the TM5 zooming algorithm has been shown. Results that are calculated with a uniform resolution of 3° × 2° closely resemble those in which more half of the grid is coarsened to 9° × 6° resolution. Thus, high-resolution simulations become feasible. It is intended to compare these simulations to observations from measurements campaigns and satellite instruments in the (lower) stratosphere.

Acknowledgement. The authors wish to express their gratitude to the HALOE team for providing us with their observations. We thank the other members of the TDLAS and MkIV teams, especially I. H. Howieson, N. R. Swann and P. T. Woods from the National Physical Laboratory. B. Steil, Ch. Brühl from the Max Planck Institute for Chemistry in Mainz and J. Greenblatt, at Princeton University, are thanked for fruitful discussions. We also thank A. Segers and P. van Velthoven from the Royal Netherlands Meteorological Institute for providing the software to process the meteorological fields. B. Bregman is funded by the EC project TOPOZ III EVK2-CT-2001-00102.

ACPD

3, 2261–2284, 2003

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ACPD

3, 2261–2284, 2003

The impact of model grid zooming on tracer transport

M. M. P. van den Broek et al.

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ACPD

3, 2261–2284, 2003

Table 1. An overview of the different horizontal resolutions used in this study

	Region 1 (global) lon × lat	Region 2 (zoom) lon × lat
Gl_96	9° × 6°	
Gl96_NH32	9° × 6°	3° × 2° (24° N–90° N)
Gl_32	3° × 2°	
Gl32_NP11	3° × 2°	1° × 1° (30° N–90° N)

ACPD
3, 2261–2284, 2003

The impact of model grid zooming on tracer transport

M. M. P. van den Broek et al.

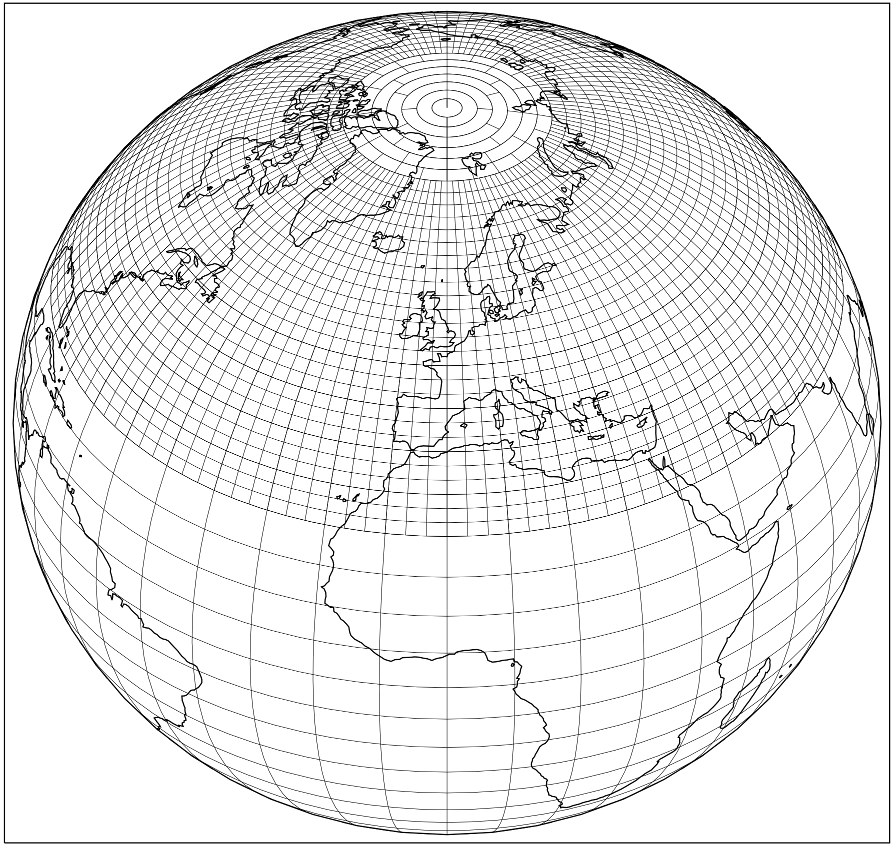

Fig. 1. An illustration of the horizontal zoom grid of TM5. Zoom option GI96_NH32 is shown here.

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3, 2261–2284, 2003

The impact of model grid zooming on tracer transport

M. M. P. van den Broek et al.

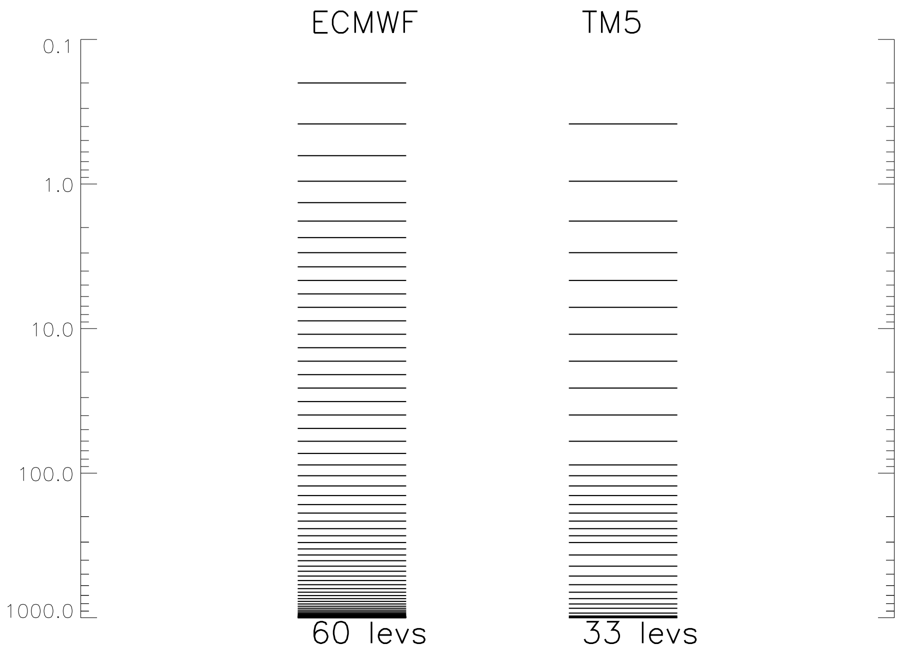

Fig. 2. The vertical grid of TM5 and the original ECMWF vertical grid.

ACPD
3, 2261–2284, 2003

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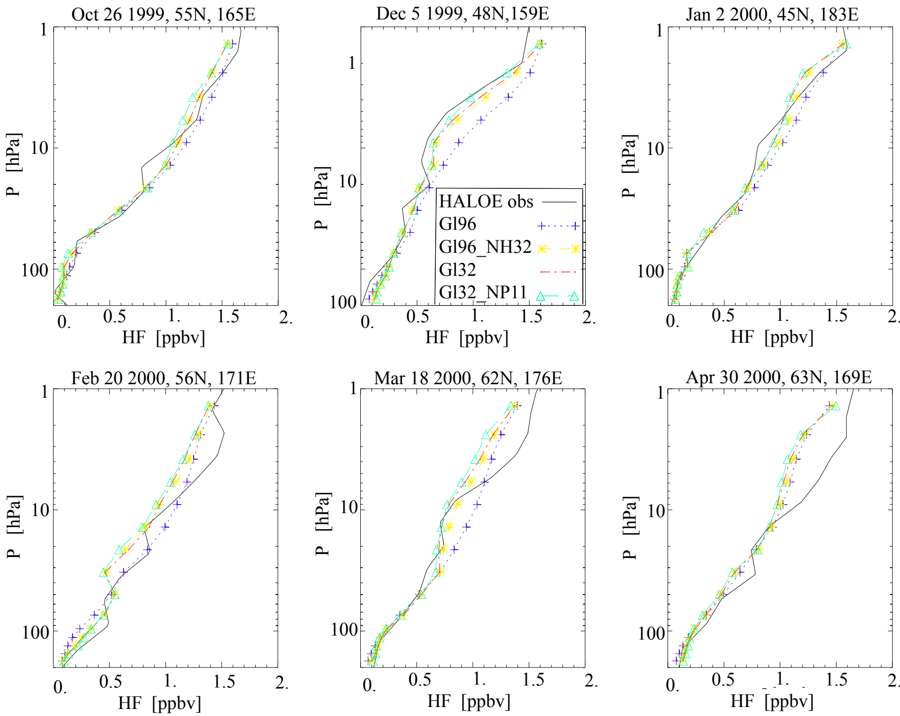

Fig. 3. Modeled HF [ppbv] compared to HALOE profiles outside the polar vortex on 26 October and 5 December 1999 and 2 January, 20 February, 18 March and 30 April 2000.

ACPD
3, 2261–2284, 2003

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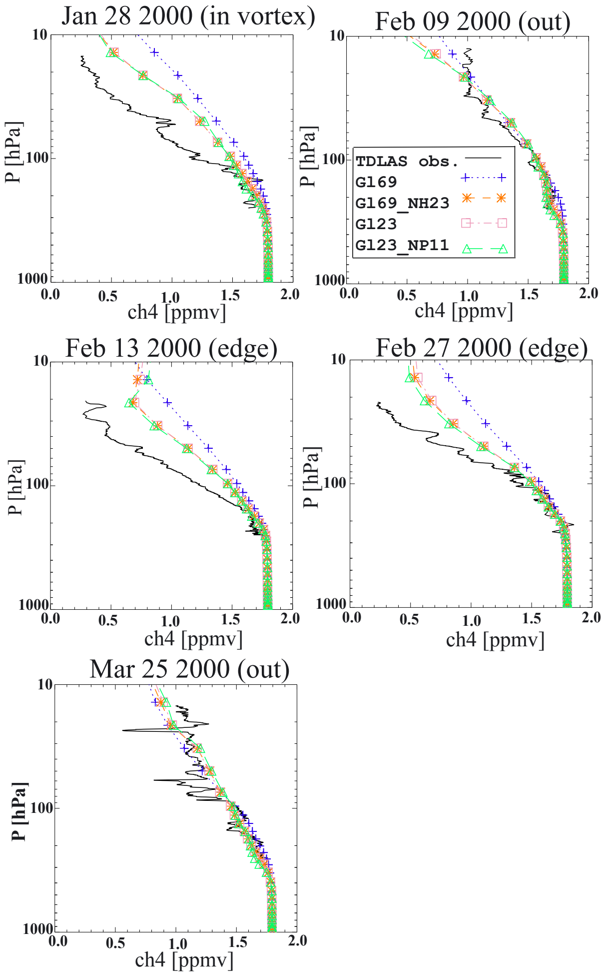

Fig. 4. Modeled CH_4 [ppmv] compared to TDLAS profiles, on 27 January, 9, 13 and 18 February and 25 March 2000.

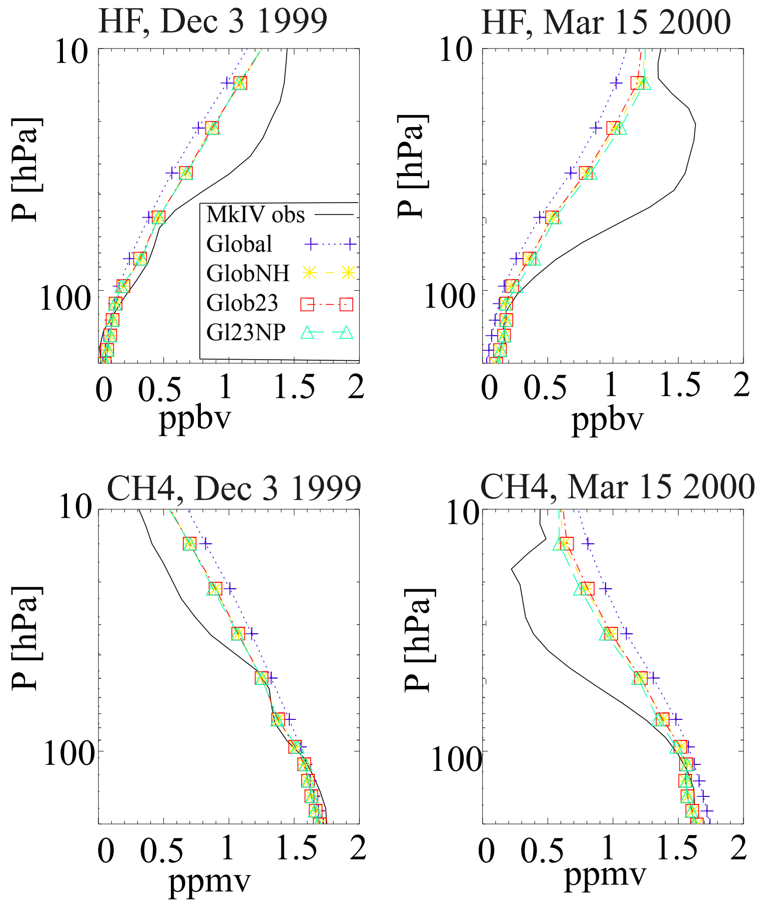

Fig. 5. Modeled HF [ppbv] and CH_4 [ppmv] compared to MkIV profiles on 3 December 1999 and 15 March 2000.

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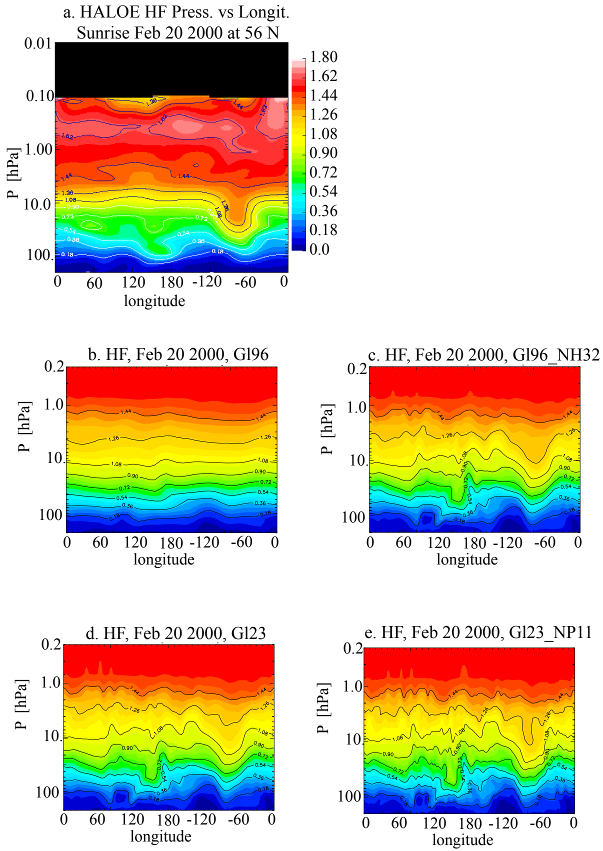

Fig. 6. Modeled HF [ppbv] compared to HALOE observations on 20 February 2000, longitudinal cross section at 56° N.

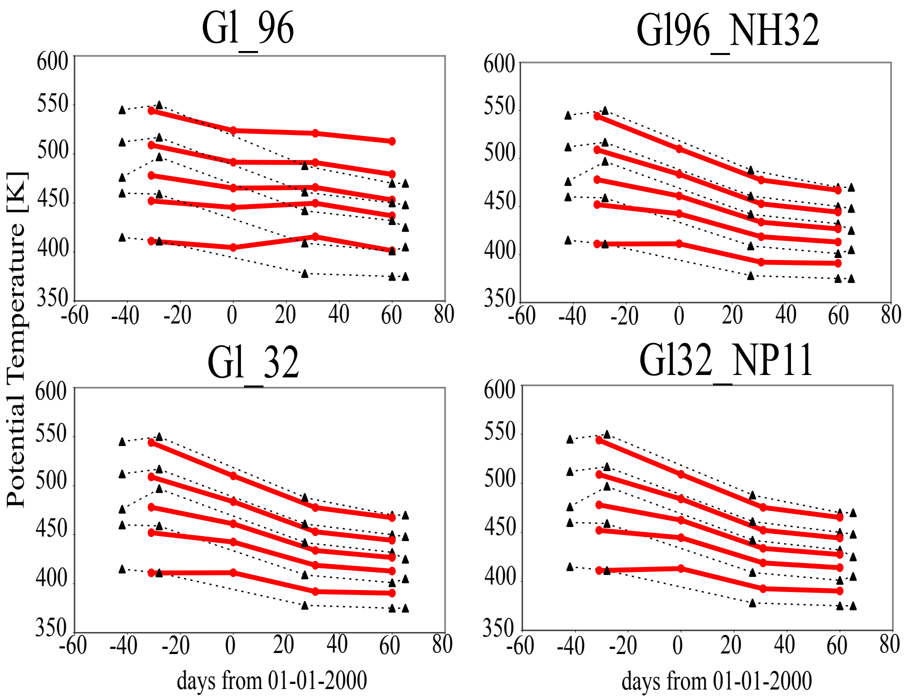

Fig. 7. Potential temperature throughout the winter of 1999–2000 along CH4 isopleths for observations (Greenblatt et al., 2002) in black-dotted lines, with the triangles representing the profile observations, and for model results on each first day of the month (red circles connected by solid lines) from all zooming options.