Energetic particle precipitation in ECHAM5/MESSy1 – Part 1: Downward transport of upper atmospheric NO\(_x\) produced by low energy electrons

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Abstract. The atmospheric chemistry general circulation model ECHAM5/MESSy1 has been extended by processes that parameterise particle precipitation. Several types of particle precipitation that directly affect NO\(_x\) and HO\(_x\) concentrations in the middle atmosphere are accounted for and discussed in a series of papers. In the companion paper, the ECHAM5/MESSy1 solar proton event parametrisation is discussed, while in the current paper we focus on low energy electrons (LEE) that produce NO\(_x\) in the upper atmosphere. For the flux of LEE NO\(_x\) into the top of the model domain a novel technique which can be applied to most atmospheric chemistry general circulation models has been developed and is presented here. The technique is particularly useful for models with an upper boundary between the stratopause and mesopause and therefore cannot directly incorporate upper atmospheric NO\(_x\) production. The additional NO\(_x\) source parametrisation is based on a measure of geomagnetic activity, the A\(_p\) index, which has been shown to be a good proxy for LEE NO\(_x\) interannual variations. HALOE measurements of LEE NO\(_x\) that has been transported into the stratosphere are used to develop a scaling function which yields a flux of NO\(_x\) that is applied to the model top. We describe the implementation of the parametrisation as the submodel SPACENOX in ECHAM5/MESSy1 and discuss the results from test simulations. The NO\(_x\) enhancements are shown to be in good agreement with independent measurements. A\(_p\) index data is available for almost one century, thus the parametrisation is suitable for simulations of the recent climate.

1 Introduction

Since the 1980’s measurements and models have shown that under certain circumstances, NO\(_x\) produced in the thermosphere by precipitating low energy electrons (LEE) can be transported downward into the stratosphere and there engage in catalytic ozone destruction (Brasseur and Solomon, 1986; Callis et al., 1998; Callis and Lambeth, 1998; Callis et al., 2001, 2002; Randall et al., 2007; Funke et al., 2005). There is emerging evidence that this is an important process amongst several sun-earth connection mechanisms (e.g. Rozanov et al., 2005). The electrons originate at the sun and from magnetospheric reservoirs, and precipitate at high latitudes during times of enhanced geomagnetic activity. In terms of stratospheric NO\(_x\) production, Funke et al. (2005) found electrons with energies up to approximately 30 keV, which deposit their energy above 90 km, to be the most relevant. There they lead to the production of NO\(_x\) through dissociation and ionization processes (Rusch et al., 1981). In the polar winter, where the photochemical loss of NO\(_x\) is negligible and where the Brewer-Dobson circulation leads to a downward transport, NO\(_x\) enhancements can be transported down into the stratosphere and lead to significant ozone loss. This has been termed the energetic particle precipitation (EPP) indirect effect by Randall et al. (2007), in contrast to the EPP direct effect where NO\(_x\) and HO\(_x\) are produced in the middle atmosphere mainly through highly energetic electrons and protons.

Measurements of enhancements of NO\(_x\) formed by low energy electrons (LEE NO\(_x\)) have been made by a growing number of instruments. The Limb Infrared Monitor of the Stratosphere (LIMS) observed NO\(_2\) mixing ratios of up to 175 ppbv in the 1978/1979 winter (Russell et al., 1988). The fact that such enhancements of NO\(_x\) occur on a regular basis was realized when the Halogen Occultation Experiment (HALOE) data became available. Such observations
are for example described in Siskind et al. (2000), Hood and Soukharev (2006) and Randall et al. (2007). Other studies of this type include Randall et al. (1998), who showed NO\textsubscript{2} enhancements using the Polar Ozone and Aerosol Measurement (POAM II) instrument and Rinland et al. (1999), who reported polar winter NO\textsubscript{2} descent seen by the Atmospheric Trace Molecule Spectroscopy (ATMOS) instrument on board the space shuttle.

An extensive study using the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) on board ENVISAT by Funke et al. (2005) clearly showed NO\textsubscript{x} enhancements in the 2003 Southern Hemisphere winter stratosphere with mixing ratios of up to 200 ppbv. Seppälä et al. (2007) used GOMOS and POAM III measurements to show that the descent of LEE NO\textsubscript{x} can be a major contributor to stratospheric NO\textsubscript{x} enhancements also in the Northern Hemisphere.

Only recently studies have been able to argue conclusively that stratospheric NO\textsubscript{x} enhancements due to LEE are linked to geomagnetic activity. Such results are for example presented in Siskind et al. (2000), Hood and Soukharev (2006), and Randall et al. (2007). As a measure for global geomagnetic activity often the A\textsubscript{p} index is employed. The A\textsubscript{p} index is derived from magnetic field component measurements at 13 subauroral geomagnetic observatories (Mayaud, 1980).

In addition to geomagnetic activity, meteorological conditions can have a significant effect on the amount of NO\textsubscript{x} found in the polar stratosphere. A stronger and better isolated polar vortex enhances the descent of NO\textsubscript{x} from the mesosphere and thermosphere. Especially in the Arctic, where dynamical variability is greater than in the Southern Hemisphere, this can occasionally lead to pronounced NO\textsubscript{x} enhancements that are not linked to geomagnetic activity, as has been shown by Randall et al. (2006).

Treatment of an additional NO\textsubscript{x} source in the mesosphere and thermosphere in models has been neglected apart from very few sensitivity studies. Siskind et al. (1997) used a two-dimensional chemical transport model which included E-region chemistry and an ionization source due to auroral particles. However, problems with the model dynamics prevented a good agreement with HALOE data. A very recent study by Vogel et al. (2008) shows Arctic Winter 2003/04 ozone loss resulting from mesospheric NO\textsubscript{x}. The CLaMS model in combination with MIPAS satellite data were employed and a significant impact on stratospheric ozone as well as on total column ozone were found. An idealised NO\textsubscript{x} source in the upper mesosphere representing relativistic electron precipitation (REP) was implemented into the Freie Universität Berlin Climate Middle Atmosphere Model with online chemistry (FUB-CMAM-CHEM) by Langemat et al. (2005). Although the source was likely to be overestimated, the results showed that the mechanism is important for ozone chemistry. A positive response was reported for ozone at high latitudes at 40–45 km, and a negative response for the tropical lower stratosphere.

Here, we describe a simple parametrisation for NO\textsubscript{x} produced by LEE for use in atmospheric chemistry general circulation models (AC-GCMs). The combination of the Modular Earth Submodel System (MESSy) and the general circulation model ECHAM5 is briefly introduced in Sect. 2.1. Due to the fact that the upper boundary of ECHAM/MESSy (EMAC) in the MA (middle atmosphere) setup is located at 0.01 hPa, the AC-GCM is well suited for this study. The parametrisation and its implementation in EMAC in form of the submodel SPACENOX are described in Sect. 2.2. The evaluation and the discussion of the results are presented in Sect. 3.

2 Model description

2.1 ECHAM5/MESSy1

The ECHAM/MESSy Atmospheric Chemistry (EMAC) model is a numerical chemistry and climate simulation system that includes submodels describing tropospheric and middle atmosphere processes and their interaction with oceans, land and human influences (Jöckel et al., 2006). It uses the first version of the Modular Earth Submodel System (MESSy1) to link multi-institutional computer codes. The core atmospheric model is the 5th generation European Centre Hamburg general circulation model (ECHAM5, Roeckner et al. (2006)). The model has been shown to consistently simulate key atmospheric tracers such as ozone (Jöckel et al., 2006), water vapour (Lelieveld et al., 2007), and lower and middle stratospheric NO\textsubscript{x} (Brühl et al., 2007). For the present study we applied EMAC (ECHAM5 version 5.3.01, MESSy version 1.6) in the T42L90MA-resolution, i.e. with a spherical truncation of T42 (corresponding to a quadratic gaussian grid of approximately 2.8 by 2.8 degrees in latitude and longitude) with 90 vertical hybrid pressure levels up to 0.01 hPa. This part of the setup matches the model evaluation study by Jöckel et al. (2006). Enabled submodels are also the same as in Jöckel et al. (2006) apart from the new submodels SPE and SPACENOX, a more detailed treatment of the solar variation in the photolysis submodel JVAL, and the submodel FUBRad (Nissen et al., 2007), a high-resolution short-wave heating rate parametrisation. The submodel SPE is described in the companion paper (Baumgaertner et al., 2009), SPACENOX is described here. The chosen chemistry scheme for the configuration of the submodel MECCA1 (Sander et al., 2005) is simpler compared to the configuration in Jöckel et al. (2006). For example, the non-methane hydrocarbon chemistry is not treated at the same level of detail. The complete mechanism is documented in the supplement to this paper at http://www.atmos-chem-phys.net/9/2729/2009/acp-9-2729-2009-supplement.zip.

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2.2 The submodel SPACENOX

The focus of this work is to study the interannual variability of LEE NO$_x$ and its temporal and spatial behavior during the polar winter. Randall et al. (1998), Randall et al. (2007) and Siskind et al. (2000) have shown that the $A_p$ index is in general sufficient to describe measured interannual variations in the southern polar vortex. Neither seasonal nor interannual variations of the transport between the source region and the model top, i.e. the lower thermosphere (LT), can be captured if the $A_p$ index is used as the only input variable. Seasonal variations of this transport are in the model parametrised using a sinusoidal time dependency (see below). Interannual variations of transport in the LT are not considered, based on the fact that a good agreement between interannual variations of $A_p$ and stratospheric NO$_x$ enhancements was found by the authors mentioned above, and because of the lack of a long term dataset for vertical transport in the lower thermosphere.

In the mesosphere, which is mostly captured by the model, and the stratosphere, variations in the strength of the Southern Hemisphere polar vortex are known to be small, but any interannual variations present in the model do not correlate with observed vortex strength because the model simulations presented here are not relaxed to observations. Other forcings, such as sea surface temperatures and chemistry boundary conditions, are not sufficient to reproduce observed vortex variability, such as the sudden warming in 2002.

For the Northern Hemisphere, where dynamic variability is much more pronounced than in the Southern Hemisphere, less evidence exists for a simple relationship between the $A_p$ index and stratospheric NO$_x$ enhancements. Therefore, emphasis here will be on the Southern Hemisphere, while aspects with respect to the implementation of the parametrisation for the Northern Hemisphere as well as results from that area will only be discussed briefly.

Because of the observed direct relationship between the $A_p$ index and NO$_x$ enhancements, the $A_p$ index was chosen as the only required time-varying input for the parametrisation.

In order to obtain the measured NO$_x$ mixing ratios in the model stratosphere, the $A_p$ index needs to be scaled appropriately to yield the required NO flux at the model top. Estimates of NO$_x$ produced in the thermosphere and transported downward into the southern polar stratosphere have been derived from HALOE measurements by Randall et al. (2007), hereafter referred to as R07. Their results cover the years 1992 to 2005 and thus cover more than one solar cycle. This is probably the longest time series of such measurements available. It encompasses the entire spectrum of geomagnetic activity and the $A_p$ index, which has been shown to have a superimposed variation of the time scale of the length of the solar cycle.

In order to develop a scaling function for the flux at the model top, the $A_p$ index was averaged over the period from May to July to yield annual mean values. This time series was fitted to the amount of average annual excess NO$_x$ below 45 km presented in R07 (their Fig. 9), derived there from deviations from the standard low NO$_x$ versus low CH$_4$ relation. Using a least squares fitting algorithm this yields the function

$$ f_{\text{LEE--NOX}}(A_p) = A_p^{2.5} \cdot 1.04 \times 10^{-3} \cdot \text{GM}. \quad (1) $$

Note that since $A_p$ is dimensionless the scaled result is multiplied by 1 GM to yield LEE NO$_x$ with unit giga moles (GM). Figure 1 (top) depicts the May-July average $A_p$ index, Fig. 1 (bottom) shows LEE NO$_x$ derived using Eq. (1) (black) and average annual LEE NO$_x$ after R07 (red). The good agreement indicates that in the Southern Hemisphere the interannual variability of the downward transport in the polar vortex is small, so that almost all of the variability can be explained by the variations in geomagnetic activity.

In order to derive a flux of NO$_x$, excess NO$_x$ densities need to be considered. Similar to above, the scaling function is derived using the data from R07. Because the time resolution of the flux is desired to be higher than yearly, the $A_p$ index was averaged over 2-week periods in order to be compatible with the results from R07 Fig. 7, reproduced here as Fig. 6. Then, $A_p^{2.5} \cdot a \text{ \ cm}^{-3}$ was fitted to yearly maximum values of R07 Fig. 7 yielding $a = 2.20 \cdot 10^7$. Then excess NO$_x$ densities $g_{\text{LEE--NOX}}$ are

$$ g_{\text{LEE--NOX}}(A_p) = A_p^{2.5} \cdot 2.20 \times 10^5 \text{\ cm}^{-3}. \quad (2) $$

For the flux calculation the following information is needed: (1) excess densities $g_{\text{LEE--NOX}}$, (2) an average vertical velocity, (3) a loss factor which accounts for transport out of the polar night region. Instead of making assumptions about the latter two, which would be error-prone, a trial-and-error approach was chosen in order to get results at 45 km
that match the observations. Therefore, a value for the combination of the latter factors was established through a series of test simulations. Several EMAC simulations with a variable factor $c$ (see Eq. 3) were conducted for the year 2003 in lower vertical resolution with 39 levels (T42L39, model top also at 0.01 hPa). Model excess NO$_x$ densities at 45 km were calculated by subtracting densities from a reference simulation with the submodel turned off. Then, model excess NO$_x$ were compared to the results of R07 (their Fig. 7). The required flux was then determined to be

$$ F = A_p^{2.5} \cdot c \cdot 2.20 \times 10^5 \text{cm}^{-2} \text{s}^{-1} $$

(3)

where $c=0.23$ for “average excess NO$_x$” (see Fig. 6, or Fig. 7 of R07) and $c=0.45$ for “maximum excess NO$_x$”.

The transport to lower altitudes only acts at high latitudes during winter. Therefore, the flux needs to be constrained to a high-latitude region and be modulated as a function of time of the year. Because of a lack of data describing the seasonal variation of vertical velocities in the lower thermosphere, the following time dependency was chosen:

$$ F = A_p^{2.5} \cdot c \cdot 2.20 \times 10^5 \text{cm}^{-2} \text{s}^{-1} \cdot \max (0.1, \cos(\pi/182.625 \cdot (d - 172.625))) $$

(4)

where $d$ is day of year. This sinusoidal variation centered around solstice represents the minimum requirement of a seasonal variation with maximum in winter. The 10% flux in summer was estimated from HALOE measurements at 0.01 hPa, which indicate elevated NO$_x$ levels during high geomagnetic activity even in summer. A restriction with respect to the latitudes where the flux is applied can be chosen via the Fortran95 namelist of the submodel. There have been findings that enhancements occur down to 30–40° latitude (Siskind et al., 1997). However, Funke et al. (2005) showed that in the middle atmosphere the enhancements are confined to the vortex (their Figs. 5, 6, 7). Therefore we have here used a minimum absolute latitude of 55° representing a conservative estimate. Also possible would be a geomagnetic activity dependent latitudinal extent which has been suggested in the past, but because of other uncertainties this is not likely to improve the results significantly.

In principle, Eq. (4) can be used for any time resolution of the $A_p$ index. Although there has not been any evidence presented that $A_p$ correlates with excess NO$_x$ in the upper mesosphere on shorter time scales, it is very likely that LEE NO$_x$ will follow geomagnetic activity also on shorter timescales than yearly. On the other hand, because of the transport timescales involved (assuming 1 km/day, the transport e.g. from 110 km to 80 km would take 30 days), a resolution higher than approximately one month is unlikely to improve the results. Here, the flux $F$ is calculated from monthly mean values of $A_p$. The estimated flux is distributed in the form of NO over the top two model levels in order to avoid strong gradients and other undesired effects that could result from introducing the flux into only the top layer, which acts as a sponge layer in the model.

It should be noted that measurements of stratospheric NO$_x$ are only available for a limited number of years. The geomagnetic $A_p$ index in comparison has been measured since 1932 and reconstructions are possible even further into the past (Nagovitsyn, 2006). Therefore, the fact that the presented parametrisation only requires the $A_p$ index as an input function, and is not relying on satellite measurements, is of great advantage for model simulations spanning several decades.

A method often used to prescribe boundary conditions for different types of long-lived gases is to nudge the tracer to a known mixing ratio. In principle, using HALOE data this method would have been feasible to implement. However, the described emission of the tracer is preferable in this case, because otherwise other processes that influence NO$_x$ mixing ratios are overwritten.

In order to assess the capability of the model and the parametrisation to reproduce NO$_x$ mixing ratios in the Northern Hemisphere, the parametrisation was applied there also.

![Fig. 2. MIPAS IMK/IAA (a) and EMAC (b) CO mixing ratios (ppmv) inside the southern polar vortex during the Southern Hemisphere winter 2003. The vortex edge was defined using the Nash criterion. The white contour lines denote the altitude in km. (a) reproduced from Funke et al. (2005) with kind permission from AGU and B. Funke.](image-url)
Although the scaling function given by Eq. (3) was developed on the basis of NO$_x$ enhancements in the southern polar region, no changes were made to the parametrisation. Only the time dependency (Eq. 4) was shifted by six months:

$$F = A_p^{2.5} \cdot 2.20 \times 10^5 \text{cm}^{-2} \text{s}^{-1} \cdot \max (0.1, \cos(\pi/182.625 \cdot (d - 355.25))).$$

(5)

The validity of this approach is discussed further in the following section.

3 Results and discussion

In general, the submodel SPACENOX and EMAC can be applied in different setups. In this paper, we will only be concerned with simulations where measured $A_p$ indices are prescribed and the GCM is free running, i.e. the meteorology is not relaxed towards the observed meteorology. Only in this configuration it is possible to perform simulations for many decades, as reliable information on global meteorology only became available with the start of the satellite era. However, as mentioned earlier, the dynamical conditions are an important factor in controlling the amount of NO$_x$ that reaches the stratosphere. Since in this model setup the meteorology, and especially the properties of polar air descent, will be different to the actual meteorology, care needs to be taken when interpreting the results.

In order to evaluate the technique and the submodel, a simulation covering the period 1992 to 2003, forced by corresponding sea surface temperatures and sea-ice coverage, is discussed. From 1992 to September 2002 the “average excess NO$_x$” scaling, after that the “maximum excess NO$_x$” scaling was applied as described above. First, the model results for the geomagnetically very active Southern Hemisphere winter 2003 are described and compared to satellite based measurements. Aspects that are addressed include the descent of air inside the polar vortex and characteristics of the LEE NO$_x$. Then, the interannual variability of LEE NO$_x$ is discussed, and effects on ozone and other constituents are mentioned. Finally, the effects of the parametrisation applied in the Northern Hemisphere are evaluated.

3.1 Southern Hemisphere

3.1.1 Vertical transport

Carbon monoxide, which in the middle atmosphere is mainly produced by photodissociation of CO$_2$, is used here to show that the model reproduces the general features of vertical transport in the Antarctic. Model results are compared to data from the MIPAS instrument on board ENVISAT, initially presented by Funke et al. (2005), hereafter referred to as F05. MIPAS CO, retrieved by the IMK/IAA (Institut für Meteorologie und Klimaforschung/Instituto de Astrofisica de Andalucia) processor, in the polar vortex is shown as a function of time and potential temperature in Fig. 2a (reproduced from F05 Fig. 4c), and corresponding model results are shown in Fig. 2b. In general, the prevailing descent of air maximising in early winter is reproduced by the model. At potential temperatures above 1500 K agreement is good throughout the winter, however, at lower altitudes and starting in June model CO mixing ratios are too high, indicating that the downward transport is too strong. The implications for the NO$_x$ transport will be discussed later where appropriate. The reasons for this discrepancy are subject to investigations independent of the work presented here.

3.1.2 LEE NO$_x$ in 2003

Figure 3 depicts the simulated mixing ratios of NO$_x$ south of 60°S during 2003. Strong enhancements with mixing ratios of more than 300 ppbv are evident in the mesosphere. They are related to the NO$_x$ produced by the SPACENOX submodel due to the large $A_p$ index during most of the southern winter 2003 (see Fig. 1). Also clearly distinguishable is a sudden enhancement at the end of October. This is related to the solar proton event and is discussed in the companion paper (Baumgaertner et al., 2009). The latitudinal extent of the NO$_x$ enhancements in the Southern Hemisphere winter 2003 is shown in the lower two panels of Fig. 4. In June mixing ratios of more than 200 ppbv extend from the South Pole to 60°S. In the upper stratosphere in August, NO$_x$ enhancements of up to 20 ppbv still reach 60°S. This indicates that NO$_x$ is confined by the polar vortex as expected and will be discussed in more detail below.

Southern polar stratospheric enhancements of NO$_x$ due to downward transport from the upper atmosphere have been presented by F05 using MIPAS measurements for the winter 2003, reproduced here as Fig. 5a. Since these measurements did not form a basis for the parametrisation in any form, the comparison is independent. In order to ease a comparison with F05, potential temperature was chosen as vertical coordinate. This also allowed a consistent transformation to equivalent latitude (Nash et al., 1996). Transformed onto an equivalent latitude, potential vorticity increases (decreases)
monotonically towards the north (south) pole. This allows a simple determination of the position of a grid box with respect to the edge of the polar vortex. Averaging over regions of high equivalent latitude means only small regions of air outside of the vortex are included. In addition, the vortex edge was calculated from the potential vorticity gradient according to Nash et al. (1996). With this it was possible during every model output timestep to determine the average mixing ratios inside the polar vortex.

NOx mixing ratios inside the polar vortex are shown in Fig. 5b. Geopotential height was converted to an approximate geometric altitude and is shown as white contours. Downward transport of a NOx enhancement exceeding 45 ppbv in June/July is clearly discernable and is generally in good agreement with the MIPAS observations with respect to magnitude, timing, and altitude of the enhancements. A NOx enhancement centered around 2500 K in August is only found in the model results and does not appear in the MIPAS data. Examining the CO abundances inside the vortex, Fig. 2a and b, reveals that in the model a strong descent of mesospheric air occurred during this time, leading to the NOx enhancements. The MIPAS CO measurements do not show this feature, explaining the difference between model and observed NOx at this time. As mentioned earlier, the CO measurements and model results also differ below 1500 K from June onwards, with the model showing stronger descent than observed. This difference also explains the higher NOx mixing ratios in late winter below 1500 K.

3.1.3 LEE NOx interannual variability

To assess the interannual variability of LEE NOx, the model results from a simulation covering 1992 to 2003 are compared to the results from R07. Different to the comparison with MIPAS, these data are not independent since the parametrisation was build upon this data. The data for October 2002 to November 2003 are the same as discussed above, however, for 1992 to September 2002 the “average excess NOx” scaling (see Sect. 2.2) was applied. Therefore, only half of the amount of NOx was emitted into the model top. Figure 7 of R07, reproduced here as Fig. 6, shows excess NOx densities at 45 km derived from HALOE data for 1992 to 2005 in 2-week time periods. Since HALOE derived densities in R07 ideally represent estimates for the...
Fig. 6. Maximum (solid) and average (dotted) excess NO\textsubscript{x} densities derived from HALOE. Reproduced from Randall et al. (2007) with kind permission from AGU and C. Randall.

Fig. 7. EMAC excess NO\textsubscript{x} densities inside the Southern Hemisphere polar vortex at 45 km. Note that for 1992–2002 the “average excess NO\textsubscript{x}” scaling was applied, in 2003 the “maximum excess NO\textsubscript{x}” scaling. The vortex edge was defined using the Nash criterion.
entire vortex region, we have at first not sampled the model output at HALOE measurement locations. Instead NO\textsubscript{x} densities were averaged over the area of the polar vortex and averaged in 2-week time periods in accordance with R07. In order to approximate excess densities, 0.75 \times 10^8 \text{cm}^{-3} was subtracted from the absolute densities, which yielded almost no excess NO\textsubscript{x} in the years where none is expected due to very low geomagnetic activity. The resulting EMAC excess densities are depicted in Fig. 7. A large interannual variability is evident. Almost no excess NO\textsubscript{x} is seen in the years 1993, 1997, and 1999, while large amounts are found in 1994, 2000, and 2003. This is in agreement with the May-July A\textsubscript{p}-index (Fig. 1), as expected. There is also a qualitative agreement with excess densities shown in Fig. 6. In a number of years, quantitative agreement is also good. In 2003 maximum excess densities of up to 7 \times 10^8 \text{cm}^{-3} were derived in R07, where the model shows between 6 and approximately 9 \times 10^8 \text{cm}^{-3}. Therefore, in 2003 there is good agreement with the maximum excess densities from R07. In the other years, when the “average excess NO\textsubscript{x}” scaling was applied, the model agrees better with the average excess densities from R07. However, R07 considered the results based on the maximum excess densities more reasonable. In the light of the good agreement between MIPAS NO\textsubscript{x} and the model simulation for 2003 with the “maximum excess NO\textsubscript{x}” scaling, this conclusion by R07 is further corroborated.

Concerning a comparison of the temporal behavior of the model excess densities with the results shown in Fig. 6, systematic discrepancies are found. As evident for example in the year 1995, elevated levels of NO\textsubscript{x} density in R07 are found until early August, whereas model densities are usually only elevated until early July. There are several possibilities to explain these differences. First, in the model we prescribed a temporal behavior using a cosine function of time of the year, centered on solstice as described above. This means that statistically NO\textsubscript{x} production is largest in June. However, due to the power-law dependency, this is unlikely to be the cause for the large fall-off after the end of June. For example, in 1995, this is clearly attributable to the change in A\textsubscript{p}-index: In May (June, July, August) the average A\textsubscript{p}-index was 18.6 (10.2, 7.7, 9.4). Instead, the time shift could mean that the time for the vertical transport between the source region and the model lid cannot be neglected as is done here. This also means that the source region is likely to be significantly higher than the model lid which is located at 0.01 hPa. Introducing a time lag between the A\textsubscript{p}-index and the NO\textsubscript{x} injection might therefore improve the results and will be subject of future work. A second possible explanation lies in the HALOE sampling as a function of latitude. Until July HALOE measures only up to approx. 50° S, so it only captures NO\textsubscript{x} enhancements near the vortex edge and misses the much larger enhancements towards the pole, as discussed by R07. In late winter, the sampling includes latitudes up to 70° S and thus also captures larger NO\textsubscript{x}, but at least in some years (e.g. 1995) the bulk of the NO\textsubscript{x} enhancements has already been transported to lower altitudes. The convolution of these two aspects could lead to a distorted apparent temporal behavior, i.e. underestimate early winter enhancements and overestimate late winter enhancements, possibly leading to a relatively monotonous enhancement as seen in Fig. 6 in 1995.
A direct point-to-point comparison between model and HALOE (Version 19) NO\textsubscript{x} was therefore performed additionally. For this, the model output was sampled at HALOE NO\textsubscript{x} measurement locations and at 45 km altitude. Then, normalised histograms were computed for periods of low (winters of 1996, 1997, 1999, 2001, 2002) and high (winters of 1992, 1994, 2000, 2003) geomagnetic activity separately. Finally, the differences between each pair of histograms from the two periods were calculated. The resulting percentage change histograms are shown for HALOE and EMAC in Fig. 8, left and right, respectively. As expected, a shift from lower to higher NO\textsubscript{x} values during high geomagnetic activity is evident in both the HALOE data and the model. However, the shift is more pronounced in the observations, again indicating that the applied “average excess NO\textsubscript{x}” scaling underestimates NO\textsubscript{x} production.

Some of the features evident in Fig. 7 are related to Solar Proton Events. For example, the sudden increase in NO\textsubscript{x} density in July 2000 lead to densities up to \(11 \times 10^8\) cm\(^{-3}\). It is interesting to note that the enhancement in R07 is only half as large. The Solar Proton Event parametrisation is discussed in the companion paper, therefore such features are not discussed further in the present study.

### 3.1.4 Effects on ozone

Due to the fact that NO\textsubscript{x} can engage in catalytic ozone destruction, in the stratosphere significant effects on ozone can be expected during winters with high geomagnetic activity. Therefore EMAC results for the year 2003, where large amounts of NO\textsubscript{x} were transported into the southern polar region, are shown here. In Fig. 9 (top panel) the change of ozone mixing ratio inside the polar vortex with respect to the result from a simulation with the submodel SPACENOX switched off is depicted. Depletion of up to 40% follows the downward transport of NO\textsubscript{x} as seen in Fig. 5. The bottom panel of Fig. 9 shows the total column ozone loss which is also strongly influenced by dynamics. A loss of between 10 and 30 DU appears to be attributable to LEE NO\textsubscript{x}. It has to be noted, however, that the overestimation of descent in the polar vortex that was deduced from the CO comparison and also seen in the NO\textsubscript{x} comparison potentially implies that the ozone loss is overestimated.

### 3.1.5 Other effects

Other members of the NO\textsubscript{y} family are likely to be affected by the NO\textsubscript{x} enhancements. Stiller et al. (2005) provided MIPAS measurements of strong HNO\textsubscript{3} enhancements inside the polar vortex during the Southern Hemisphere winter of 2003. EMAC results for HNO\textsubscript{3} in the same period are smaller by more than one order of magnitude. Since the relevant gas-phase reactions are included in the simulation (see supplement), this indicates that the measured HNO\textsubscript{3} enhancements are likely to result from ion cluster reactions (for more details see Stiller et al., 2005, and the companion paper) that are currently not included in EMAC.

### 3.2 Northern Hemisphere

For the Northern Hemisphere, where dynamical variability is much larger than in the Southern Hemisphere, additional aspects need to be considered. The larger dynamical variability has a stronger influence on the amount of LEE NO\textsubscript{x} deposited in the stratosphere (see e.g. Randall et al., 2005). Variability in the lower thermosphere is not captured in the model simulations and is thus potentially a significant error source. Concerning the upper stratosphere and mesosphere, NO\textsubscript{x} transport is exposed to the variability in the model. Therefore, since the model is free running and not reproducing observed dynamical interannual variations, the agreement between model and observed NO\textsubscript{x} is worse than by just comparing \(A\textsubscript{p}\) and measured excess NO\textsubscript{x}. On the other hand, if the model reproduces the observed dynamical
variability (e.g. by relaxing model meteorology to observed meteorology), the agreement between model and observed NO\textsubscript{x} will be better than by just comparing \( A_p \) and measured excess NO\textsubscript{x}. In the case of the presented model simulations, the model is forced with observed sea surface temperatures, an observed Quasi-Biennial Oscillation (QBO), and observed solar UV radiation. It has been shown by (e.g. Labitze, 2005) that solar and QBO forcing determine a significant fraction of interannual variability of the vortex, especially the number of mid-winter warmings. This implies that the interannual variability of the Northern Hemisphere vortex in the presented model simulations should show similar features as the observed variability. However, this is still under investigation and beyond the scope of this paper.

The latitudinal extent of LEE NO\textsubscript{x} is shown in Fig. 4 for December and February during the Northern Hemisphere winter 2002/03. Mixing ratios up to 100 ppbv are evident from the north pole to 70° N, small enhancements are found up to 40° N. Enhancements in December reach down to 2 hPa.

In order to assess the model’s capability to reproduce Northern Hemisphere NO\textsubscript{x} mixing ratios, potentially affected by LEE NO\textsubscript{x}, we carried out comparisons with satellite data similar to the approach employed for the Southern Hemisphere. F05 also presented measurements from the Northern Hemisphere winter 2002/03. NO\textsubscript{2} nighttime abundances as a function of equivalent latitude and potential temperature are depicted in their Fig. 12 (top) and are reproduced here as Fig. 10. NO\textsubscript{2} enhancements last from November to February, interrupted by stratospheric warmings. They clearly result from downward transport and reach peak mixing ratios of 16 ppbv. EMAC NO\textsubscript{2} mixing ratios for the same period are shown in Fig. 11. Note that the nighttime MIPAS NO\textsubscript{2} only represent a lower limit for NO\textsubscript{x}.

Both the model and observations show a strong descent of NO\textsubscript{x} starting at 3000 K in November, with mixing ratios of more than 16 ppbv. The excess NO\textsubscript{x} is transported down to altitudes of 1500 K (40 km) during the following two months. A second strong enhancement observed by MIPAS in December is not captured by the model. In February, both model and observations again show enhancements above 2500 K, exceeding 16 ppbv in the observations and reaching 10 ppbv in the model. Because of the fact that the main features of the observed NO\textsubscript{2} enhancements are reproduced, we conclude that the parametrisation also works well under moderate dynamical conditions in the Northern Hemisphere, similar to those found in the 2002/2003 winter. Note that the lower altitude enhancements found from January onwards have been shown to be related to midlatitude air that was transported to higher latitudes (see F05), resulting in NO\textsubscript{2} mixing ratios of up to 10 ppbv that last at least until April 2003.

A variety of dynamical conditions can be captured by comparing model NO\textsubscript{x} with HALOE observations. Similar to above, normalised NO\textsubscript{x} histograms for periods of high (winters of 1991/1992, 1992/1993, 1993/1994, 1994/1995) and low (winters of 1995/1996, 1996/1997, 1997/1998) geomagnetic activity are subtracted and shown in Fig. 12. In general both the HALOE and EMAC data show the shift from low to high NO\textsubscript{x} values during geomagnetically active winters, confirming the validity of the parametrisation for a wider range of dynamical conditions.

4 Conclusions

A parametrisation of the production of NO\textsubscript{x} in the thermosphere through LEE has been developed with the aim to be able to describe NO\textsubscript{x} mixing ratios in the stratospheric polar vortex. The approach is based solely on monthly mean values of the \( A_p \) index, which has been shown to be a good proxy for Southern Hemisphere interannual variations of vortex NO\textsubscript{x} mixing ratios. A scaling function was developed based on published interannual variations of LEE NO\textsubscript{x} derived from HALOE measurements. The technique allows to quantitatively capture measured NO\textsubscript{x} enhancements in the stratosphere that are due to LEE precipitation in the thermosphere. The implementation in EMAC was evaluated against independent NO\textsubscript{x} measurements by MIPAS for the geomagnetically very active Southern Hemisphere winter 2003 as well as the moderately active Northern Hemisphere winter 2002/03. Excellent agreement was found for both periods. For the Southern Hemisphere winter 2003 a significant impact on ozone was shown. The presented parametrisation of LEE NO\textsubscript{x} is therefore a valuable addition to the EMAC AC-GCM and will be useful for simulations of the recent climate. Because the \( A_p \) index is available since 1932, it is possible to quantify interannual variability on timescales even longer than satellite measurements of NO\textsubscript{x} enhancements due to

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**Fig. 12.** Same as Fig. 8 but for latitudes north of 40° N. Left: HALOE, right: EMAC.
LEE. Combined with model implementations of other solar activity dependent processes, namely photolysis, radiative heating, and SPEs, it will be possible to study the holistic impact of solar activity variations on the Earth’s atmosphere. Results from an EMAC simulation encompassing these processes and covering the period 1960 until 2003 are in preparation for publication. Due to the success of the technique seen in the presented evaluation and its proven significance on polar ozone chemistry, it is recommended to include such a parametrisation into middle atmosphere AC-GCMs.

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