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New dynamic NNORSY ozone profile climatology

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Abstract

Climatological ozone profile data are widely used as a-priori information for total ozone using DOAS type retrievals as well as for ozone profile retrieval using optimal estimation, for data assimilation or evaluation of 3-D chemistry-transport models and a lot of other applications in atmospheric sciences and remote sensing. For most applications it is important that the climatology represents not only long term mean values but also the links between ozone and dynamic input parameters. These dynamic input parameters should be easily accessible from auxiliary datasets or easily measureable, and obviously should have a high correlation with ozone. For ozone profile these parameters are mainly total ozone column and temperature profile data. This was the outcome of a user consultation carried out in the framework of developing a new, dynamic ozone profile climatology.

The new ozone profile climatology is based on the Neural Network Ozone Retrieval System (NNORSY) widely used for ozone profile retrieval from UV and IR satellite sounder data. NNORSY allows implicit modelling of any non-linear correspondence between input parameters (predictors) and ozone profile target vector. This paper presents the approach, setup and validation of a new family of ozone profile climatologies with static as well as dynamic input parameters (total ozone and temperature profile). The neural network training relies on ozone profile measurement data of well known quality provided by ground based (ozonesondes) and satellite based (SAGE II, HALOE, and POAM-III) measurements over the years 1995–2007. In total, four different combinations (modes) for input parameters (date, geolocation, total ozone column and temperature profile) are available.

The geophysical validation spans from pole to pole using independent ozonesonde, lidar and satellite data (ACE-FTS, AURA-MLS) for individual and time series comparisons as well as for analysing the vertical and meridian structure of different modes of the NNORSY ozone profile climatology. The NNORSY ozone profile climatology is available to the community as a comprehensive software library.

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1 Introduction

Ozone is one of the most important trace gases in the atmosphere. Through its strong absorption of ultraviolet (UV) radiation it also influences the vertical profile of atmospheric temperature. The correlation between ozone and temperature profile has been widely studied by multiple linear regression analysis (Steinbrecht et al., 2003) with model data and from long-term total ozone observations of TOMS (Total Ozone Monitoring Spectrometer) (Bhartia, 2003) and SBUV (Solar Backscatter Ultra-Violet) instruments (Heath and Park, 1975), as well as NCEP reanalysis temperature profile data (Kistler et al., 2001). Results show global patterns of total ozone column and lower stratospheric temperature correlated with the QBO (quasi-biennial oscillation), the solar cycle, and other parameters. Other atmospheric parameters like tropopause height are also correlated with ozone profile values and shape (Steinbrecht et al., 1998). Further studies of Steinbrecht et al. (2006) yield a quantification of major modes of interannual variation of total ozone column and lower stratospheric temperature from long-term observations and reanalysis as well as from coupled chemistry and climate models.

Several available ozone profile climatologies are based on lookup tables. For construction of the SUNYA climatology of the State University of New York (Wang et al., 1995) total ozone column values based on TOMS from 1978 to 1992, stratospheric profiles based on SAGE II (Stratospheric Aerosol and Gas Experiment-II) from 1984 to 1992 and ozonesonde data were used. The stratospheric vertical distribution is based on the data of SAGE II which provides data up to 60 km at 1 km resolution from October 1984 to November 1989. The resulting data set consists of monthly zonal means with 59 pressure levels from 0.28 hPa to 1000 hPa.

The UGAMP ozone climatology (Li and Shine, 1999) describes the 4-dimensional distribution of ozone, and it has been built by combining several data sets from satellite observations (SBUV, SAGE II, SME, TOMS) as well as ozonesonde data covering five years (1985 to 1989). It provides monthly means of the ozone column as well as 5-yr

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averages on a 2.5° × 2.5° horizontal grid, with 47 levels ranging from the ground up to 0.001 hPa.

Monthly zonal mean ozone profiles for 17 zonal bands (80° S–80° N) are provided by the ozone profile climatology developed by Fortuin and Kelder (1998). Ozonesonde data from 30 different stations as well as data from SBUV, SBUV/2 and TOMS for the period of 1980 to 1991 were used to prepare the climatology. It provides ozone partial column data on 19 vertical pressure levels (1000 hPa to 0.3 hPa) and includes information about ozone profile standard deviation. A further monthly zonal mean ozone profile climatology has been prepared by NASA Goddard Space Flight Center (GSFC) (McPeters et al., 2007) based on previous work of Logan (1999) and McPeter (1997) for a tropospheric ozone climatology. It was compiled using ozone sonde data up to 24 km as well as SAGE II and UARS MLS data for the height range 29 km to 60 km and a weighted average in between. The GSFC is also authoring the TOMS V8 climatology (Barthia, 2003) which provides total ozone classified zonal mean ozone profile data for 10° latitude bands.

Total ozone dependence is also a feature of the ozone profile climatology compiled by Lamsal et al. (2004). They provide separate sets for winter/spring and summer/fall seasons, for high and mid-latitude regions. For tropical and subtropical regions no seasonal dependent profile data are available. Primarily ozone profile data sets from ozonesondes (WOUDC, 2010) including SHADOZ measurements (Thompson et al., 2003), SAGE II (Cunnold et al., 1989, 1991, 2002a, b), POAM III (Lucke et al., 1999; Lumpe et al., 2002; Randel et al., 2003) as well as National Meteorological Center (NMC) and UKMO temperature profiles in the time range 1990 to 2000 contributed to this ozone profile climatology.

Two more recent ozone climatologies are described in Mze et al. (2010) and Ziemke et al. (2011). The latter is a global climatology of tropospheric and stratospheric ozone columns derived from AURA OMI and MLS (Schoeberl et al., 2006; Levelt et al., 2006; Froidevaux et al., 2008) measurements for the period October 2004 through December 2010, while Mze uses ENVISAT/GOMOS measurements (Bertroux et al., 2000,

2004) covering 2002–2008 and compiles a monthly ozone distribution in the upper troposphere and in the stratosphere (15–50 km). Comparisons were made to eight SHADOZ stations in the altitude range from 15 km to 30 km; however the coarse spatial sampling of GOMOS and missing validaton for mid and high latitude restrict this climatology to tropical regions, while the climatology of Ziemke (2011) provides only columnar values for the troposphere and stratosphere.

Ozone profile climatology data are an important source of information in atmospheric sciences and especially within the retrieval community. For example, ann ozone profile climatology is needed as a-priori information for total ozone column retrieval using the TOMS (Bhartia, 2003), DOAS (Loyola et al., 2011), WFDOAS (Weber et al., 2005) or GodFit (Lerot et al., 2010) algorithms. The NNORSY climatology presented in this paper was developed in the framework of the GDP5 project for the purpose of retrieving ozone total columns from GOME using the GodFit approach.

Other applications in atmospheric science using an ozone profile climatology are ozone profile retrieval from satellite data by means of optimal estimation to constrain the solution according to Rogers' theory (Rogers et al., 1976; Rogers, 2000) applied e.g. by Mijling et al. (2010) or Lamsal et al. (2007), for background correction within retrieval schemes of other trace gases like CO_2 (Crevoisier et al., 2009), for data assimilation and validaton of 3-D chemistry and transport models, for several other applications or measurements of height resolved atmospheric parameters or for atmospheric correction in space-based imagery of the surface. Furthermore, stratospheric ozone and water vapour profiles are correlated to meteorological regimes. Especially in the UTLS region different weather regimes exhibit unique profile shapes for water vapour and ozone (Follette-Cook et al., 2009; Hudson et al., 2009).

All these correlations are highly non-linear between different known and unknown or hidden parameters of the atmospheric state and the ozone profile at different height levels. The above mentioned, already available ozone profile climatologies mainly use linear regression and advanced interpolation schemes (e.g. Ziemke et al., 2011) to smooth over the various spatial and temporal resolutions of the data sources used in compiling column and/or profile data into an ozone climatology. Very few available ozone climatologies use total ozone column as a predictor for the ozone profile shape (e.g. Bhartia, 2003; Lamsal et al., 2003), but none of them use temperature profile data as a predictor. With both parameters the current state of the atmosphere for which a climatological ozone profile is desired can be specified. To model correlations between dynamic input parameters (e.g. total ozone column and/or temperature profile) and a target vector (ozone profile in our case), data mining by means of machine learning techniques is an excellent approach. This was already proven with the NNORSY (Neural Network Ozone Retrieval System) scheme (Müller et al., 2002, 2003) and compared, which was used to set up the new dynamic ozone profile climatology. A detailed comparison study of NNORSY with other retrieval schemes can be found in Meijer et al. (2006).

In Sect. 2 the main results of a user consultation will be shown, before in Sect. 3 the basic approach and the ozone profile measurement data sets used are briefly described. In Sect. 4, the methods employed, the NNORSY processing scheme as well as the validation data will be specified. The pole-to-pole validation results are shown in Sect. 5 for the different climatology modes, by means of comparisons with single measurement stations, time series analysis as well as meridian ozone profile structure analysis, before we draw our conclusions in Sect. 6.

2 User consultation

In 2004, in an early stage of the development of the new NNORSY Ozone profile climatology, a user consultation was organised in the framework of the ESA-funded CHEOPS project. A questionnaire was sent to more than 1200 scientists and experts in atmospheric sciences. Feedback was given by 86 scientists from 35 different countries. A main achievement of the consultation was a better knowledge about user requirements on the temporal and spatial resolutions as well as the height resolution and ozone profile units. Each responder has to select one of multiple choices per category. The main results are summarized in Table 1.

Building on the feedback of the user consultation, the new NNORSY ozone profile climatology was developed, which features four different combinations (modes) of input parameters in order to be as flexible as possible for a wide range of potential applications (Table 2). Regarding spatial and temporal resolution there are in principle no restrictions because the new ozone profile climatology is provided as a software library that takes arbitrary space-time coordinates as input. In practice, the temporal and spatial resolution of the NNORSY ozone profile climatology is mainly dependent on the resolution of the dynamic input parameters provided by the user.

3 Approach and data used

Currently available climatologies for ozone profile data are usually based on look-up tables. User requirements show that for a new ozone profile climatology it is important to also use dynamic input parameters like total ozone and/or the temperature profile as predictors. These requirements (mainly temperature profile usage) lead to the NNORSY (Neural Network Ozone Retrieval SYstem) approach which was developed at our lab within the last decade for total ozone retrieval (Müller et al., 2002) as well as for ozone profile retrieval from the GOME (Müller et al., 2003; Meijer et al., 2006) and SCIAMACHY instruments. Recently, NNORSY was further developed and implemented for GOME-2 onboard MetOp-A as well as for combined GOME-2/IASI ozone profile retrieval (Felder et al., 2011).

For the different climatology modes various neural networks have to be trained. In the framework of several NNORSY projects for GOME, SCIAMACHY and GOME-2/IASI we built a large atmospheric profile data base with focus on ozone profiles. These data are collocated with analysis model data to add consistent temperature and pressure profile information. For the NNORSY climatology the following training data sources were used:

- Ozonesonde data:
  - WMO's World Ozone and UV Data Centre (WOUDC, 2010)
  - NASA's SHADOZ programme (Thompson et al., 2003)
- Satellite solar occultation measurement data:
  - SPOT-3 POAM-II data version 6: (Lumpe et al., 1997)
  - SPOT-4 POAM-III data version 4: (Lucke et al., 1999; Lumpe et al., 2002; Randel et al., 2003)
  - ERBS SAGE II data version 6.2: (Cunnold et al., 1989, 1991, 2002a, b)
  - UARS HALOE data version 19: (Nazaryan et al., 2005; Eyring et al., 2006)

The time range of training data spans 1995 to 2007 (Fig. 1). During ingestion of data into the ZSW profile database rigorous quality checks are carried out, similar to the ones described by Hassler et al. (2008) with some extensions described below. Before the data are used for neural network training, statistics on the whole training dataset are calculated for each profile level and only data within the 99 % percentile on each level are used for training. For climatology applications of ozone profiles, there is no point in trying to model very exceptional situations. Within the profile database each profile is collocated with temperature profiles from the GEOS-4 reanalysis (Bloom et al., 2005). All data are being interpolated to 61 height levels centred on 0.5 km up to 60.5 km with a sampling of 1 km. For additional quality control of ozone profiles, the temperature profile data often measured together with the ozone profile data and delivered within most original data sources are cross-checked against the GEOS-4 temperature profile data. If the deviation between both temperature profiles is too large, the whole profile is flagged as questionable and not used for successive training or validation. Various comparisons showed that if the T-profile data of the measurement data source exhibits high deviations from T-profile analysis data then the ozone profile measurement is usually of poor quality. Figure 2 shows the temporal and spatial distribution of the

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ozone profile data used, while in Fig. 3 latitudinal histograms of ozone profile data from the different sources are displayed. It shows for instance that for WOUDC more data are available in the Northern Hemisphere while POAM data are only available for higher latitudes.

For setting up a climatology, the seasonal dependence is also important. In Fig. 4 this dependence of the ozone profile measurements used for training is shown by data source. Only for POAM II the histogram shows significantly more data in the second half of the year. The influence on the overall distribution is quite small because the absolute amount of data from the other limb sounders like SAGE, HALOE and POAM III is much higher.

A common feature of limb sounder data is the poor quality of profile retrievals around and below the tropopause region. During ingest of limb sounder ozone profile data into the training database, all ozone profile data at and below the tropopause were flagged and not used for successive neural network training. The tropopause was calculated from GEOS-4 reanalysis data using a mixture of WMO lapse rate definition and 2.5 PVU surfaces.

4 Neural network training

The neural networks for different climatology modes were trained separately using the same number of training patterns. The problem to overcome for training climatology modes with total ozone column input parameter was that no independent measurements of the total ozone column for each ground and satellite ozone profile measurement (training pattern) were available. Total ozone column measurements from satellites like GOME, GOME-2, TOMS or OMI were ruled out because their retrieval algorithms already use different ozone profile climatologies and/or model data, and we would like to avoid any possible feedback loop to already existing ozone profile climatologies.

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Therefore we first trained the neural network for climatology mode TLLT (Table 2) which already gives a very good estimate of the ozone profile. For this training we did not split up the ozone profile measurement database for training, test and evaluation. This neural network training for mode TLLT was used to supplement the missing parts of ozone profiles for a given data source (e.g. above burst point for ozonesondes and below tropopause for limb sounder data). After supplementing missing ozone profile levels with first neural network climatology for mode TLLT, the total ozone column was calculated by integrating the resulting ozone profiles. This total ozone column value was later on used for training of modes TLLO and TLLTO where it is used as input parameter. For training of the neural networks, the ozone profile database was divided into training and test dataset. For a first validation during development mainly ACE-FTS, and AURA-MLS ozone profile data were used which were not part of the training or test data. With this setup, all four NNORSY climatology modes were trained and tested. Figure 5 shows the training results for climatology mode TLLO as an example. For full geophysical validation, additional sonde and lidar measurements from NDACC stations are used which will be described in the next section.

5 Validation

The validation of the new climatology relies on independent ground-based and satellite ozone profile measurements. The ground-based data comprise ozonesonde and lidar observations associated with the Network for the Detection of Atmospheric Composition Change (NDACC, formerly NDSC, Kurylo and Zander, 2001) with pole-to-pole coverage for the time range 1996 to 2009. Satellite-based ozone profile data of global ACE-FTS and AURA-MLS measurements in the time frame 2004 to 2009 cover the altitude range above the tropopause, which leads to an overlap region between tropopause and about 30 km for ozonesonde data and about 45 km for lidar data. Prior to the comparison, the ground-based ozone profiles from ozonesonde and lidar are smoothed vertically to the estimated resolution of the NNORSY climatology

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of 3 km FWHM (Müller et al., 2003) and are interpolated to the standard NNORSY height grid with 1 km sampling. In parallel to the validation of the NNORSY climatology, the ozone profile climatology used for the TOMS Version 8 ozone column retrieval algorithm (Bhartia, 2003) was compared to the same correlative dataset.

5.1 Individual comparisons at single stations

Validations started with the analysis of comparisons at all individual ground stations, for dynamic climatology mode TLLO using total ozone as input parameter. The example given in Fig. 6 also includes ozone profile data of the TOMS V8 climatology (Bhartia, 2003), since it is based on the same predictors. Figure 6 shows that for the selected stations from four different regions, the overall agreement of NNORSY ozone profiles with sonde data is good. However, in ozone hole conditions the NNORSY as well as the TOMS V8 climatology do not represent the full extent of the high ozone depletion around 20 km altitude, which is expected because the corresponding ozonesonde measurements show that the ozone concentration is almost zero. In the tropical stratosphere the TOMS V8 climatology profile at ozone peak altitude is too low while NNORSY is in good agreement with the sonde measurements. A similar pattern can be observed for the measurement at Uccle station where TOMS V8 climatology is lower than NNORSY, but the smoothed ozonesonde measurement falls around the mean at ozone peak levels, which also shows the smoothing effect for both climatologies very well.

Figure 7 shows the vertical structure of the statistical agreement of NNORSY (mode TLLO) and TOMS V8 climatology at the same stations already used in Fig. 6. At Nairobi NNORSY underestimates ozone in the height range of 10–20 km and overestimates it ~10 % below 10 km. The largest underestimation up to 30 % is at 18 km. At this height level there are very steep gradients of the ozone profile and for example only a slight shift of 0.5 km in the height assignment can cause such a bias. Below this height the ozone concentration is very low and therefore the absolute deviation is small. The statistics for Neumayer Station in the Antarctic show an underestimation of NNORSY

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around 10 km altitude while TOMS V8 shows an overestimation in the height range of 6–9 km. For Uccle station the agreement of NNORSY is very good while TOMS V8 exhibits an overestimation of up to 30 % around 10 km altitude.

5.2 Time series

Comparisons over time were performed against satellite measurement data (ACE-FTS V2.2 and AURA-MLS V2.3) as well as against single stations providing ozonesonde and lidar measurements. The comparisons with satellite data were carried out and averaged in 5 degree latitude bands. Figures 8 to 11 show comparisons for the time range mid 2004 to end 2009 for NNORSY mode TLLO. Figure 8 displays AURA-MLS and ACE-FTS latitude band 75° N–70° N for the arctic region and Fig. 9 for mid latitude Northern Hemisphere (50° N–45° N). For the tropical region only AURA-MLS data are used because the orbit of ACE-FTS does not allow solar occultation measurements within the tropics (Fig. 10). Figure 11 represents comparisons for Antarctic region (65° S–70° S). The laminar structures in the comparisons with MLS, which are most pronounced in the tropics (Fig. 10) and getting weaker towards higher latitudes, originate from the MLS measurement data and are not a feature of the NNORSY climatology. This was confirmed by comparisons of MLS data with HALOE measurements for the years 2004–2005 (not shown) and reported back to the PI group of AURA-MLS at JPL (L. Froidevaux, personal communication, 2011).

In the mesosphere comparisons with ACE-FTS show a negative bias of up to 20 % while the comparisons with AURA-MLS show a positive bias of 10–20 % above 50 km. These differences can partly be explained by the diurnal cycle of ozone concentration and the other part seems to be stem for some kind of scan pattern bias in the AURA-MLS data itself which can also be seen in direct comparisons of MLS data with HALOE V19 data.

Figure 12 shows mean difference time series for ozonesonde and lidar measurements for different climatological regions ranging from the arctic station Ny-Alesund to Neumayer station in the Antarctic, as well as mid latitude station Uccle and lidar

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measurements from Mouna Loa (tropics), for NNORSY climatology mode TLLO. The agreement for Mouna Loa is very good in the stratosphere but show some negative bias in tropopause while for Ny-Alesund and Uccle the main differences can be seen in the UTLS region and for Neumayer station during ozone hole conditions in the altitude range between 10 km–20 km, where the absolute ozone concentration can be very low inducing very steep gradients in the ozone profile (Fig. 6). Therefore the smoothing error can be a major contribution to the overall difference shown.

A negative bias can be recognized in the inter-tropical UTLS region around 18 km (Fig. 10), and around 10 km in the polar regions (Fig. 12). For the high and mid-latitude regions the agreement between measurement and NNORSY climatology is within 10 % while in the inter-tropical zone standard deviation is higher (Fig. 7).

5.3 Meridional structure and total ozone sensitivity

In order to compare the four different modes of the NNORSY climatology qualitatively and quantitatively, Fig. 13 shows the meridional structure for all climatology modes. It can be seen that modes with (TLLO, TLLTO) and without (TLL, TLLT) total ozone as predictor are more similar and that the agreement with total ozone used as predictor is better. The NNORSY mode TLL does not use any dynamic input parameter and therefore this climatology generates ozone profiles only dependent on date and geographical location.

Figures 14 and 15 show a sensitivity study with respect to the total ozone input parameter dependent on latitude for the Southern and Northern Hemisphere, respectively. The interval for varying the total ozone input parameter is dependent on latitude and the plots will give an indication for the valid range of total ozone input for the NNORSY climatology.

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6 Conclusions

This paper reports on the development and verification of a new generation ozone profile climatology based on the NNORSY approach. In order to study the geophysical soundness of the climatology, output ozone profiles have been compared to correlative measurements acquired by a network of ground-based ozonesonde and lidar stations deployed from pole to pole. The quantitative and qualitative agreements between the climatology and ground-based observations resemble those reported for the first NNORSY ozone profile retrievals for ERS-2/GOME (Müller et al., 2003). A monthly mean agreement often better than ±10 % is obtained in the stratosphere and the inter-percentile 68 % is close to 10 %. For ozone hole conditions the NNORSY climatology has a positive bias in situations where ozone concentration in the 20 km altitude range is very low. The better comparison results obtained when smoothing the ozonesonde and lidar data at 3 km resolution confirm this value as a good estimate of the NNORSY vertical resolution.

In general the different climatology modes have similar agreement but the dynamic modes of the climatology – including the ozone total column and/or the temperature profile as input parameters – yield better results than the static mode TLL, mainly by reducing the standard deviation of the mean difference. Under ozone hole conditions the vertical structure of early ozone depleted profiles (September) is not reproduced well by the modes TLL and TLLT. Mode TLL strongly overestimates the ozone concentration in ozone depleted situations, while for mode TLLT the overestimation is less and at lower altitudes (Fig. 13). Especially for Antarctica modes including total ozone give much better results for ozone depleted profiles with slight overestimation at ozone depleted altitudes.

For the inter-tropical tropopause modes TLL and TLLO underestimate the ozone concentrations between 10 km and 20 km, while modes TLLT and TLLTO exhibit slight overestimation. This can be an indication that including the temperature profile as a predictor for the ozone profile helps the neural networks to implicitly estimate

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tropopause height and thus to perform a coarse airmass type classification for different climatological regimes.

If we try to compare the NNORSY ozone profile climatology to the TOMS V8 climatology, in general the relative differences between TOMS V8 and ground-based ozonesonde data are similar to those between NNORSY climatology and ground-based measurements. In the inter-tropical troposphere the TOMS V8 climatology compares better to correlative ozonesonde data than NNORSY. Positive biases are observed for TOMS V8 near the tropopause that are not present in the NNORSY climatology. This may be explained by the difference in vertical resolution between TOMS V8 using Umkehr layers and NNORSY which is estimated to ~3 km (Müller et al., 2003).

The NNORSY ozone profile climatology is available as software library as well as standalone software. The software is written in Fortran and will compile with GNU Fortran Compilers which are available on most computer system used in the atmospheric science community. This opens a broad range of applications for the NNORSY ozone profile climatology ranging from data assimilation, trace gas retrieval from satellite data as well as climate modelling tasks. Especially for total ozone column and ozone profile retrieval schemes using optimal estimation the new NNORSY ozone profile retrieval has the potential to speed up retrieval, and potentially improve retrieval results.

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References

Bertaux, J. L., Kyrola, E., and Wehr, T.: Stellar occultation technique for atmospheric ozone monitoring: GOMOS on Envisat, Earth Observation Quarterly, 67, 17–20, 2000.

Bertaux, J. L., Hauchecorne, A., Dalaudier, F., Cot, C., Kyrola, E., Fussen, D., Tamminen, J., Leppelmeier, G. W., Sofieva, V., Hassinen, S., d'Andon, O. F., Barrot, G., Mangin, A., Theodore, B., Guirlet, M., Korablev, O., Snoeij, P., Koopman, R., and Fraisse, R.: First results on GOMOS/Envisat, Adv. Space Res., 33, 1029–1035, 2004.

Bhartia, P.: Algorithm Theoretical Baseline Document, TOMS v8 Total ozone algorithm, available at: http://toms.gsfc.nasa.gov/version8/version8_update.html, 2003.

Bloom, S., da Silva, A., and Dee, D.: Technical Report Series on Global Modeling and Data Assimilation, edited by: Suarez, M. J., Documentation and Validation of the Goddard Earth Observing System (GEOS) Data Assimilation System–Version 4, NASA GSFC NASA/TM—2005–104606, 26, available at: http://gmao.gsfc.nasa.gov/systems/geos4/Bloom.pdf, 2005.

Crevoisier, C., Chédin, A., Matsueda, H., Machida, T., Armante, R., and Scott, N. A.: First year of upper tropospheric integrated content of CO_2 from IASI hyperspectral infrared observations, Atmos. Chem. Phys., 9, 4797–4810, doi:10.5194/acp-9-4797-2009, 2009.

Cunnold, D. M., Chu, W. P., Barnes, R. A., McCormick, M. P., and Veiga, R. E.: Validation Of SAGE II Ozone Measurements, J. Geophys. Res., 94, 8447–8460, 1989.

Cunnold, D. M., Zawodny, J. M., Chu, W. P., Pommereau, J. P., Goutail, F., Lenoble, J., McCormick, M. P., Veiga, R. E., Murcray, D., Iwagami, N., Shibasaki, K., Simon, P.C., and Peetermans, W.: Validation Of SAGE II NO_2 Measurements, J. Geophys. Res., 96, 12913–12925, 1991.

Cunnold, D. M., Newchurch, M. J., Flynn, L. E., Wang, H. J., Russell, J. M., McPeters, R., Zawodny, J. M., and Froidevaux, L.: Uncertainties in upper stratospheric ozone trends from 1979 to 1996, J. Geophys. Res., 105, 4427–4444, 2000a.

Cunnold, D. M., Wang, H. J., Thomason, L. W., Zawodny, J. M., Logan, J. A., and Megretskaia, I. A.: SAGE (version 5.96) ozone trends in the lower stratosphere, J. Geophys. Res., 105, 4445–4457, 2000b.

Eyring, V., Butchart, N., Waugh, D. W., Akiyoshi, H., Austin, J., Bekki, S., Bodeker, G. E., Boville, B. A., Brühl, C., Chipperfield, M. P., Cordero, E., Dameris, M., Deushi, M., Fioletov, V. E., Frith, S. M., Garcia, R. R., Gettelman, A., Giorgetta, M. A., Grewe, V., Jourdain, L., Kinnison, D. E., Mancini, E., Manzini, E., Marchand, M., Marsh, D. R., Nagashima, T., Newman, P. A., Nielsen, J. E., Pawson, S., Pitari, G., Plummer, D. A., Rozanov, E., Schraner, M., Shepherd, T. G., Shibata, K., Stolarski, R. S., Struthers, H., Tian, W., and Yoshiki, M.: Assessment of temperature, trace species, and ozone in chemistry-climate model simulations of the recent past, J. Geophys. Res., 111, D22308, doi:10.1029/2006JD007327, 2006.

Felder, M. D., Huckle, R., and Kaifel, A. K.: Synergistic Ozone Profile Retrieval from METOP GOME-2 and IASI Data, Atmos. Meas. Tech. Discuss., in review, 2012.

Follette-Cook, M. B., Hudson, R. D., and Nedoluha, G. E.: Classification of Northern Hemisphere stratospheric ozone and water vapor profiles by meteorological regime, Atmos. Chem. Phys., 9, 5989–6003, doi:10.5194/acp-9-5989-2009, 2009.

Fortuin, P. and Kelder, H.: An ozone climatology based on ozonesonde and satellite measurements, J. Geophys. Res., 103, 31709–31734, 1998.

Froidevaux, L., Jiang, Y. B., Lambert, A., Livesey, N. J., Read, W. G., Waters, J. W., Browell, E. V., Hair, J. W., Avery, M. A., McGee, T. J., Twigg, L. W., Sumnicht, G. K., Jucks, K. W., Margitan, J. J., Sen, B., Stachnik, R. A., Toon, G. C., Bernath, P. F., Boone, C. D., Walker, K. A., Filipiak, M. J., Harwood, R. S., Fuller, R. A., Manney, G. L., Schwartz, M. J., Daffer, W. H., Drouin, B. J., Cofield, R. E., Cuddy, D. T., Jarnot, R. F., Knosp, B. W., Perun, V. S., Snyder, W. V., Stek, P. C., Thurstans, R. P., and Wagner, P. A.: Validation of Aura Microwave Limb Sounder stratospheric ozone measurements, J. Geophys. Res., 113, D15S20, doi:10.1029/2007JD008771, 2008.

Hassler, B., Bodeker, G. E., and Dameris, M.: Technical Note: A new global database of trace gases and aerosols from multiple sources of high vertical resolution measurements, Atmos. Chem. Phys., 8, 5403–5421, doi:10.5194/acp-8-5403-2008, 2008.

Heath, D. F. and Park, H.: The solar backscatter ultraviolet (SBUV) and Total Ozone Mapping Spectrometer (TOMS) experiment, in The Nimbus-7 Users Guide, edited by: Madrid, C. R., Greenbelt, MD, NASA Goddard Space Flight Center, 175–211, 1978.

Hoppel, K. W., Bowman, K. P., and Bevilacqua, R. M.: Northern hemisphere summer ozone variability observed by POAM II, Geophys. Res. Lett., 26, 827–830, 1999.

Hudson, R. D., Andrade, M. F., Follette, M. B., and Frolov, A. D.: The total ozone field separated into meteorological regimes – Part II: Northern Hemisphere mid-latitude total ozone trends, Atmos. Chem. Phys., 6, 5183–5191, doi:10.5194/acp-6-5183-2006, 2006.

Kistler, R., Kalnay, E., Collins, W., Saha, S., White, G., Woollen, J., Chelliah, M., Ebisuzaki, W., Kanamitsu, M., Kousky, V., van den Dool, H., Jenne, R., and Fiorino, M.: The NCEP-NCAR 50-Year Reanalysis: Monthly Means, CD-ROM and Documentation, B. Am. Meteorol. Soc.,

82, 247–267, available at: http://www.cpc.ncep.noaa.gov/products/wesley/reanalysis.html, 2001.
Kurylo, M. J. and Zander, R. J.: The NDSC – Its status after ten years of operation, in: Proceedings of the Quadrennial Ozone Symposium 2000, Hokkaido Univ., Sapporo, Japan, edited by: NASDA, 167–168, 2001.
Lamsal, L. N., Weber, M., Tellmann, S., and Burrows, J. P.: Ozone column classified climatology of ozone and temperature profiles based on ozonesonde and satellite data, J. Geophys. Res., 109, D20304, doi:10.1029/2004JD004680, 2004.
Lamsal, L. N., Weber, M., Labow, G., and Burrows, J. P.: Influence of ozone and temperature climatology on the accuracy of satellite total ozone retrieval, J. Geophys. Res., 112, D02302, doi:10.1029/2005JD006865, 2007.
Lerot, C., Van Roozendael, M., Lambert, J.-C., Granville, J., van Gent, J., Loyola, D., and Spurr, R. J. D.: The GODFIT algorithm: a direct fitting approach to improve the accuracy of total ozone measurements from GOME, Int. J. Remote Sens., 31, 543–550, 2010.
Levelt, P. F., Hilsenrath, E., Leppelmeier, G. W., van den Oord, G. H. J., Bhartia, P. K., Tamminen, J., de Haan, J. F., and Veefkind, J. P.: Science objectives of the Ozone Monitoring Instrument, IEEE T. Geosci. Remote, 44, 1199–1208, doi:10.1109/TGRS.2006.872336, 2006.
Li, D. and Shine, K. P.: University of Reading, UGAMP Ozone Climatology, [Internet], NCAS British Atmospheric Data Centre, available at: http://badc.nerc.ac.uk/view/badc.nerc.ac.uk__ATOM__dataent_UGAMPO3, 1999.
Logan, J. A.: An analysis of ozonesonde data for the troposphere: Recommendations for testing 3-D models, and development of a gridded climatology for tropospheric ozone, J. Geophys. Res., 104, 16115–16149, 1999.
Loyola, D., Koukouli, M. E., Valks, P., Balis, D. S., Hao, N., Van Roozendael, M., Spurr, R. J. D., Zimmer, W., Kiemle, S., Lerot, C., and Lambert, J.-C.: The GOME-2 total column ozone product: Retrieval algorithm and ground-based validation, J. Geophys. Res., 116, D07302, 2011.
Lucke, R. L., Korwan, D. R., Bevilacqua, R. M., Hornstein, J. S., Shettle, E. P., Chen, D. T., Daehler, M., Lumpe, J. D., Fromm, M. D., Debrestian, D., Neff, B., Squire, M., König-Langlo, G., and Davies, J.: The Polar Ozone and Aerosol Measurement (POAM III) instrument and early validation results, J. Geophys. Res., 104, 18785–18799, 1999.
Lumpe, J. D., Bevilacqua, R. M., Hoppel, K. W., Krigman, S. S., Kriebel, D. L., Randall, C. E.,

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5, 775–812, 2012

Rusch, D. W., Brogniez, C., Ramananaherosa, R., Shettle, E. P., Olivero, J. J., Lenoble, J., and Pruvost, P.: POAM II Retrieval Algorithm and Error Analysis, J. Geophys. Res., 102, 23593–23614, 1997.
Lumpe, J. D., Bevilacqua, R. M., Hoppel, K. W., and Randall, C. E.: POAM III retrieval algorithm and error analysis, J. Geophys. Res., 107, 4575, doi:10.1029/2002JD002137, 2002.
McPeters, R. D., and Labow, G. J.: A satellite-derived ozone climatology for balloonsonde estimation of total column ozone; J. Geophys. Res., 102, 8875–8886, 1997.
McPeters, R. D., Labow, G. J., and Logan, J. A.: Ozone climatological profiles for satellite retrieval algorithms, J. Geophys. Res., 112, D05308, doi:10.1029/2005JD006823, 2007.
Meijer,Y. J., Swart, D. P. J., van der A, R. J., Baier, F., Bhartia, P. K., Bodeker, G. E., Chance, K., Erbertseder, T., Flynn, L. E., del Frate, F., Godin-Beekmann, S., Hansen, G., Hasekamp, O. P., Kaifel, A., Kelder, H. M., Kerridge, B. J., Lambert,J.-C., Landgraf, J., Liu, X., McDermid, I. S., Müller, M. D., van Oss, R. F., Pachepsky, Y., Rozanov, V., Siddans, R., Tellmann, S., Weber, M., and Zehner, C.: Evaluation of nine different GOME ozone profile algorithms, J. Geophys. Res., 111, D21306, doi:10.1029/2005JD006778, 2006.
Mijling, B., Tuinder, O. N. E., van Oss, R. F., and van der A, R. J.: Improving ozone profile retrieval from spaceborne UV backscatter spectrometers using convergence behaviour diagnostics, Atmos. Meas. Tech., 3, 1555–1568, doi:10.5194/amt-3-1555-2010, 2010.
Müller, M. D., Kaifel, A. K., Weber, M., Tellmann, S., Burrows, J. P., and Loyola, D.: Ozone profile retrieval from Global Ozone Monitoring Experiment (GOME) data using a neural network approach (Neural Network Ozone Retrieval System (NNORSY)), J. Geophys. Res., 108, 4497, doi:10.1029/2002JD002784, 2003.
Mze, N., Hauchecorne, A., Bencherif, H., Dalaudier, F., and Bertaux, J.-L.: Climatology and comparison of ozone from ENVISAT/GOMOS and SHADOZ/balloon-sonde observations in the southern tropics, Atmos. Chem. Phys., 10, 8025–8035, doi:10.5194/acp-10-8025-2010, 2010.
Nazaryan, H., McCormick, M. P., and Russell III, J. M.: New studies of SAGE II and HALOE ozone profile and long-term change comparisons, J. Geophys. Res., 110, D09305, doi:10.1029/2004JD005425, 2005.
Randall, C. E., Rusch, D. W., Bevilacqua, R. M., Hoppel, K. W., Lumpe, J. D., Shettle, E., Thompson, E., Deaver, L., Zawodny, J., Kyrö, E., Johnson, B., Kelder, H., Dorokhov, V. M., König-Langlo, G., and Gil, M.: Validation of POAM III ozone: Comparisons with ozonesonde and satellite data, J. Geophys. Res., 108, 4367, doi:10.1029/2002JD002944, 2003.

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Rodgers, C. D.: Retrieval of atmospheric temperature and composition from remote measurements of thermal radiation, Rev. Geophys., 14, 609–624, doi:10.1029/RG014i004p00609, 1976.
Rodgers, C. D.: Inverse methods for atmospheric sounding: Theory and practice, World Scientific Publishing, Singapore, 2000.
Schoeberl, M. R., Douglass, A. R., Hilsenrath, E., Bhartia, P. K., Barnett, J., Beer, R., Waters, J., Gunson, M., Froidevaux, L., Gille, J., Levelt, P. F., and DeCola, P.: Overview of the EOS Aura Mission, IEEE T. Geosci. Remote, 44, 1066–1074, 2006.
Steinbrecht, W., Claude, H., Köhler, U., and Hoinka, K. P.: Correlations between tropopause height and total ozone: Implications for long-term changes, J. Geophys. Res., 103, 19183–19192, 1998.
Steinbrecht, W., Hassler, B., Claude, H., Winkler, P., and Stolarski, R. S.: Global distribution of total ozone and lower stratospheric temperature variations, Atmos. Chem. Phys., 3, 1421–1438, doi:10.5194/acp-3-1421-2003, 2003.
Steinbrecht, W., Haßler, B., Brühl, C., Dameris, M., Giorgetta, M. A., Grewe, V., Manzini, E., Matthes, S., Schnadt, C., Steil, B., and Winkler, P.: Interannual variation patterns of total ozone and lower stratospheric temperature in observations and model simulations, Atmos. Chem. Phys., 6, 349–374, doi:10.5194/acp-6-349-2006, 2006.
Thompson, A. M., Witte, J. C., McPeters, R. D., Oltmans, S. J., Schmidlin, F. J., Logan, J. A., Fujiwara, M., Kirchhoff, V. W. J. H., Posny, F., Coetzee, G. J. R., Hoegger, B., Kawakami, S., Ogawa, T., Johnson, B. J., Vömel, H., and Labow, G.: Southern Hemisphere Additional Ozonesondes (SHADOZ) 1998–2000 tropical ozone climatology 1. Comparison with Total Ozone Mapping Spectrometer (TOMS) and ground-based measurements, J. Geophys. Res., 108, 8238, doi:10.1029/2001JD000967, 2003.
Wang, W.-C., Liang, X.-Z., Dudek, M. P., Pollard, D., Thompson, S. L.: Atmospheric ozone as a climate gas, Atmos. Res., 37, 247–256, 1995.
Weber, M., Lamsal, L. N., Coldewey-Egbers, M., Bramstedt, K., and Burrows, J. P.: Pole-to-pole validation of GOME WFDOAS total ozone with groundbased data, Atmos. Chem. Phys., 5, 1341–1355, doi:10.5194/acp-5-1341-2005, 2005.
WOUDC: ABM, & AM-IMS, & AWI-NA, & AWI-NM, & BNIHM, & CHMI-PR, & CNRS, & CWBT, & DMI, & DWD-MOHp, & DWD-MOL, & EIMO, & FMI, & FMI-SMNA, & HKO, & IMD, & INME, & INME-IZO, & INPE, & INTA, & IPSL, & JMA., & KNMI, & MDI, & ME, & MeteoSwiss, & MGO, & MMS, & MSC, & NASA-GSFC, & NASA-LaRC, & NASA-WFF, & NASDA, & NIWA, & NIWA-

LAU, & NAA-CMDL, & PIMWM, & PRLI, & RMIB, & SAWS, & SMNA, & TSMS, & U_Colorado, & U_LaReunion, & U_Nairobi, & U_Rome-CRPSM, & UAH, & UKMO, & UNKNOWN. World Ozone and Ultraviolet Radiation Data Centre (WOUDC), Data Retrieved December 2010 from http://www.woudc.org.

Ziemke, J. R., Chandra, S., Labow, G. J., Bhartia, P. K., Froidevaux, L., and Witte, J. C.: A global climatology of tropospheric and stratospheric ozone derived from Aura OMI and MLS measurements, Atmos. Chem. Phys., 11, 9237–9251, doi:10.5194/acp-11-9237-2011, 2011.

Table 1. Summary of results of the user consultation on a new ozone profile climatology. Percentages denote how often a multiple choice option was chosen, with all possible options in one category totalling 100 %.

Category	1st place	2nd place
temporal resolution	daily (40 %)	monthly (30 %)
latitudinal resolution	1° (33 %)	2.5° (30 %)
longitudinal resolution	2.5° (36 %)	5° (27 %)
height coordinates	altitude grid (45 %)	pressure levels (36 %)
additional output	standard deviation (90 %)	n/a (<10 %)
main applications (in order of picks)	(1) retrieval, (2) campaign support, (3) satellite data validation, (4) data assimilation	

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Table 2. Available input and output parameter combinations for the different modes of NNORSY ozone profile climatology.

Characteristics	Mode TLL	Mode TLLO	Mode TLLT	Mode TLLTO
Input Parameters	time, latitude, longitude	time, latitude, longitude total ozone column	time, latitude, longitude T-profile	time, latitude, longitude total ozone column T-profile
Output Parameters	O_3 Profile O_3 Profile Stdev. T-Profile T-Profile Stdev.	O_3 Profile O_3 Profile Stdev. T-Profile T-Profile Stdev.	O_3 Profile O_3 Profile Stdev.	O_3 Profile O_3 Profile Stdev.
Vertical Sampling	61 layer 1 km sampling rate			
Ozone Data Unit	ozone number density [10^{18} m^{-3}]			

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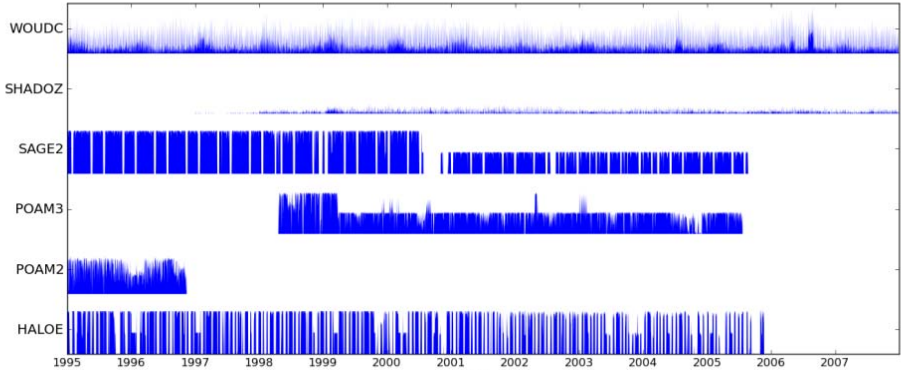

Fig. 1. NNORSY ozone profile database content used for neural network training. The vertical bars for each sensor or data source denote the relative number of measurements per day, with a common scale over all data types.

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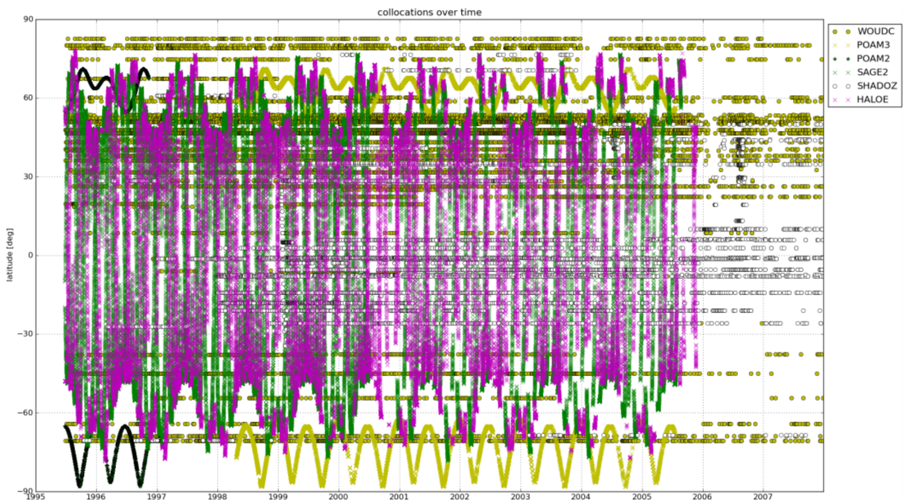

Fig. 2. Ozone profile data distribution over time and latitude. This data set is used for training neural networks for NNORSY the new ozone profile climatology.

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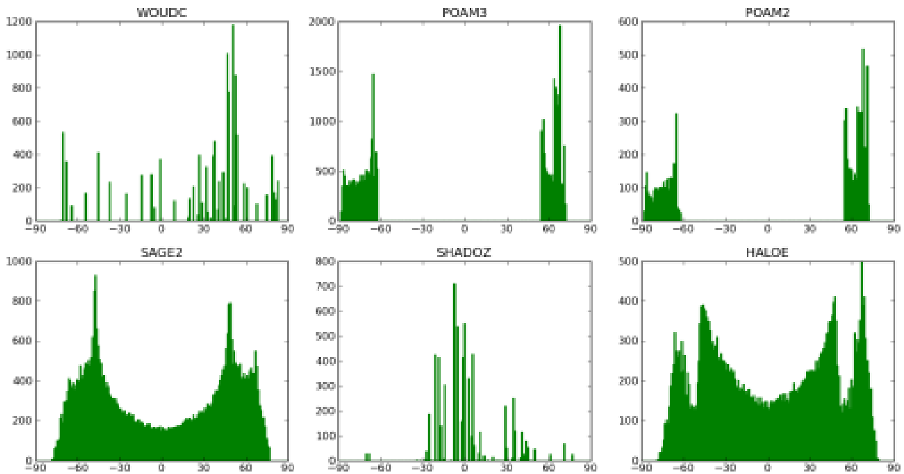

Fig. 3. Latitudinal histograms for each data source of ozone profile data used in training neural networks for the NNORSY ozone profile climatology.

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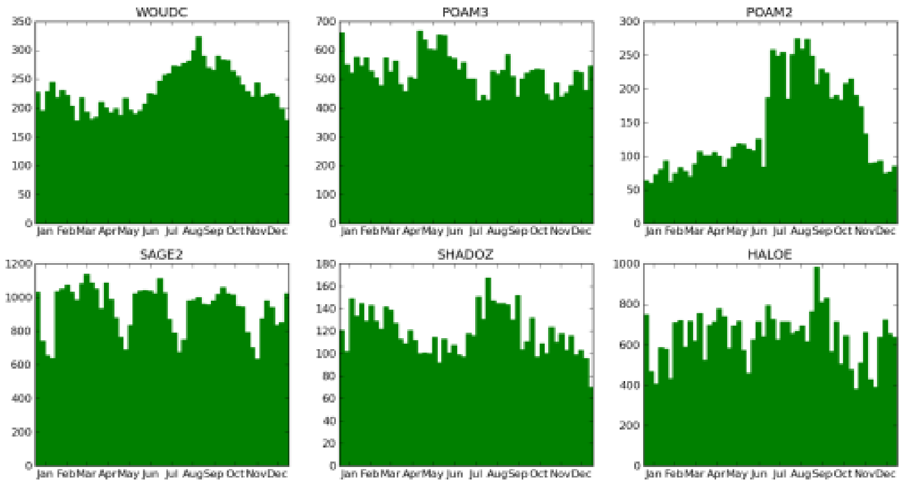

Fig. 4. Seasonal histograms for each data source of ozone profile data used for training neural networks for NNORSY ozone profile climatology. Bin size is one week.

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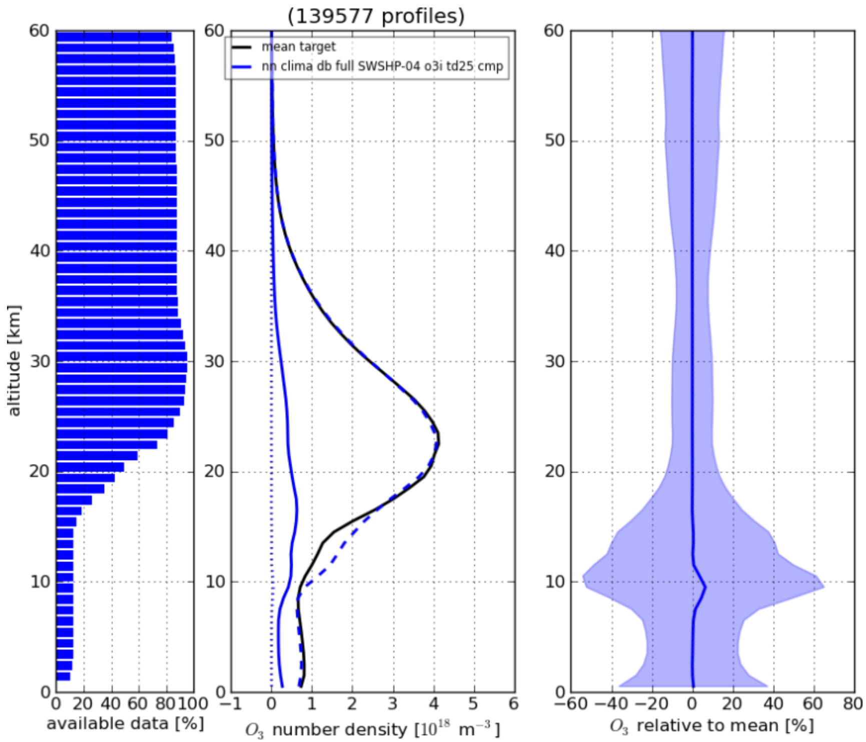

Fig. 5. Error statistics on training data set for climatology mode TLLO. In the left panel the histogram shows the relative number of available ozone profile data for each height level. In the middle panel the dotted line denotes the bias and the solid line the standard deviation. The mean profiles are calculated independently, therefore noticeable differences may occur if the number of samples at each height level is different between neural network output (dashed) and the targets (solid black). In the right panel the solid line denotes the bias and the shaded area the standard deviation.

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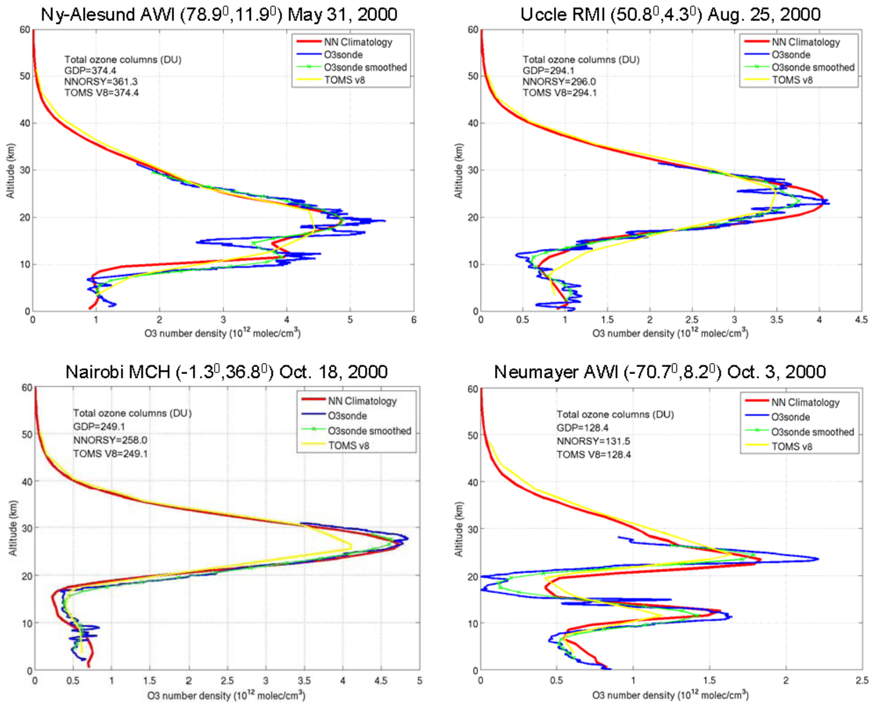

Fig. 6. Typical comparison of single profiles of NNORSY climatology mode TLLO and TOMS V8 Climatology with measurement stations in different climatological regions. Station Ny-Alesund for arctic region, Station Uccle for northern mid-latitude region, Nairobi for tropics and Neumayer for Antarctica. The red line shows NNORY climatology ozone profile, the blue line the co-located ground based raw ozone profile and the green line the same ground-based profile smoothed to estimate the NNORSY vertical resolution (3 km FWHM). The yellow line shows the corresponding TOMS V8 ozone profile. The total ozone column value in Dobson Units are results by integrating ozone profiles for NNORSY and TOMS V8 climatology while GDP denotes the total ozone retrieval of GDP Version 4.1 from ERS-2/GOME data.

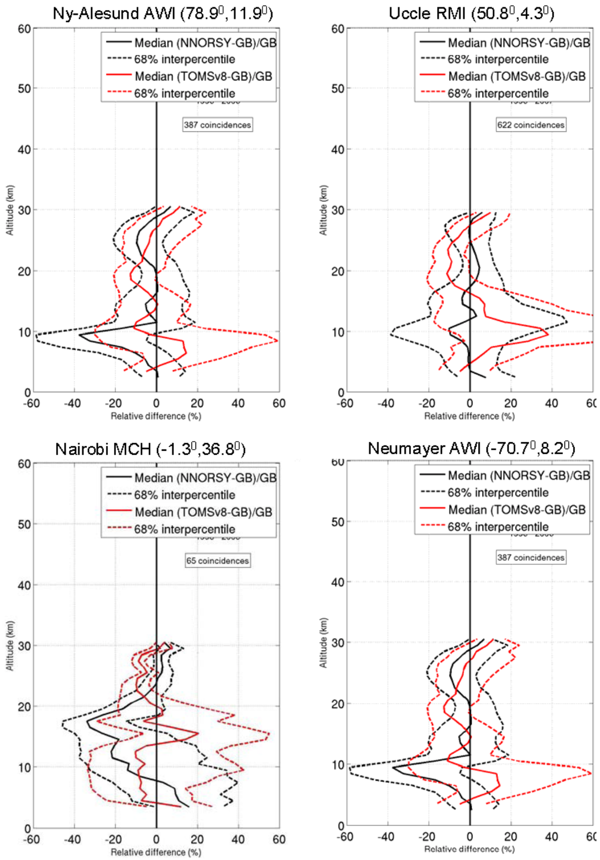

Fig. 7. Statistics between ground based (GB) ozone profile measurements and NNORSY climatology mode TLLO and TOMS V8 climatology for the stations already used in single measurement comparisons in Fig. 6.

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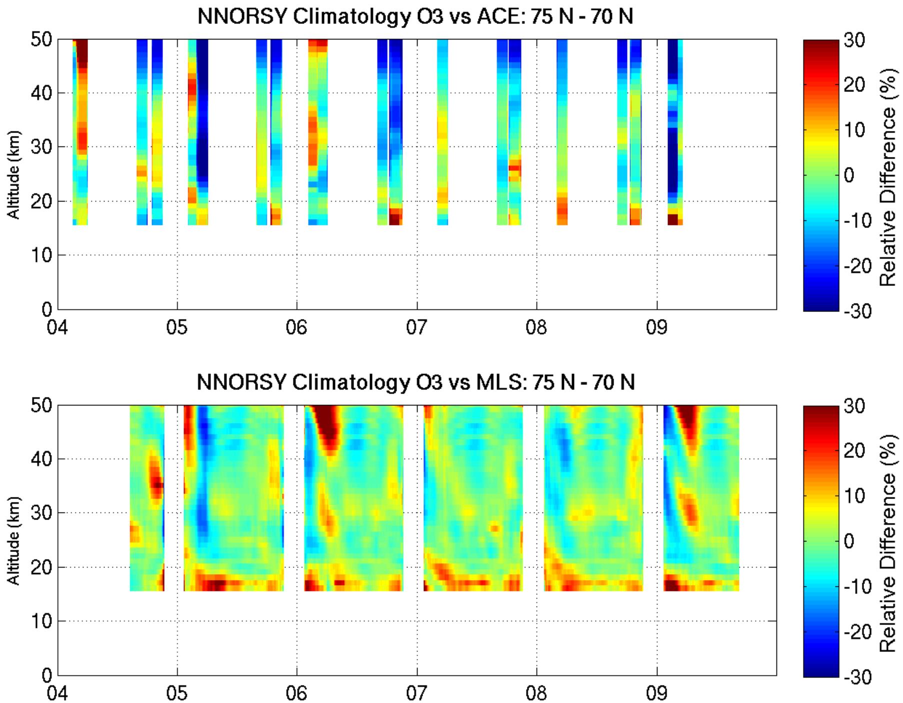

Fig. 8. Time series of the percent relative difference between the NNORSY ozone climatology (dynamic mode TLLO) in the latitude band 75° N–70° N (Artic), and the ACE-FTS and AURA-MLS data. A one month running mean has been applied to the relative difference.

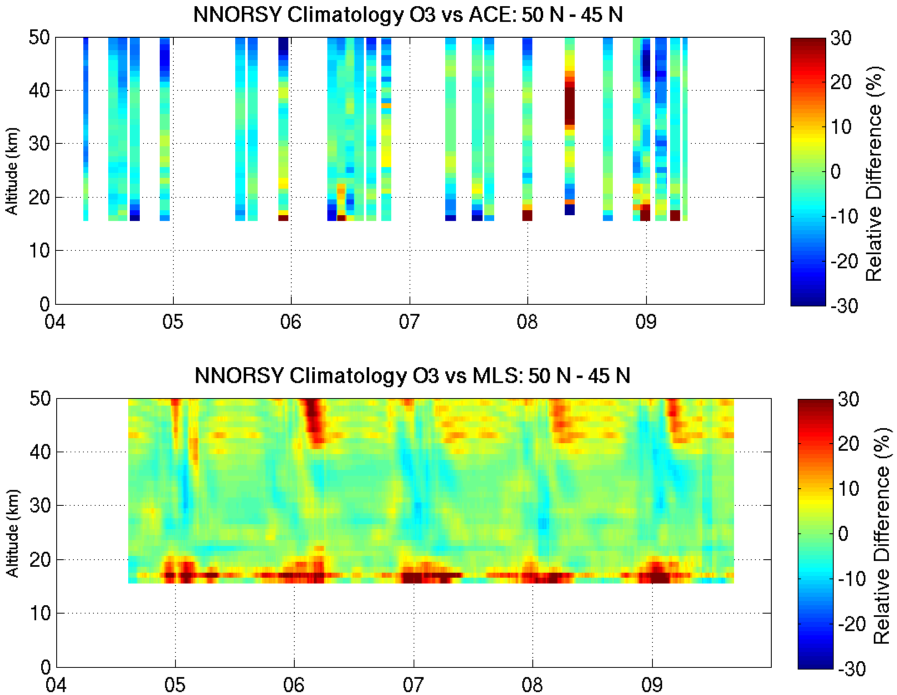

Fig. 9. Same as Fig. 8 but in the latitude band 50° N–45° N (mid latitude).

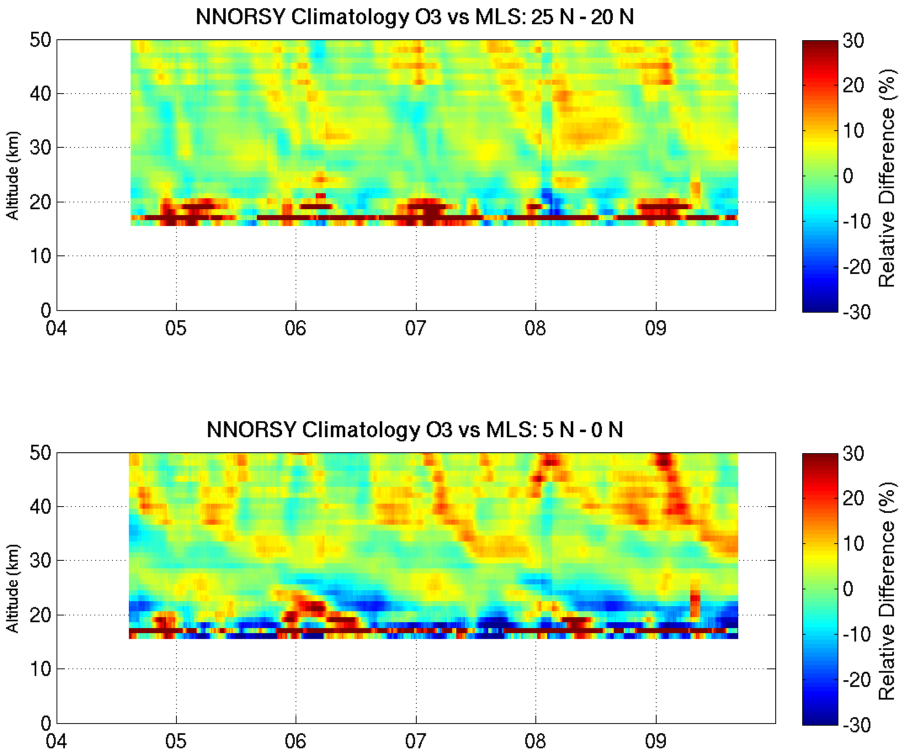

Fig. 10. Same as Fig. 8 but in the latitude band 25° N–20° N and 5° N to Equator (tropics) without comparisons for ACE-FTS data. The ACE orbit does not allow solar occultation measurements within the tropical region.

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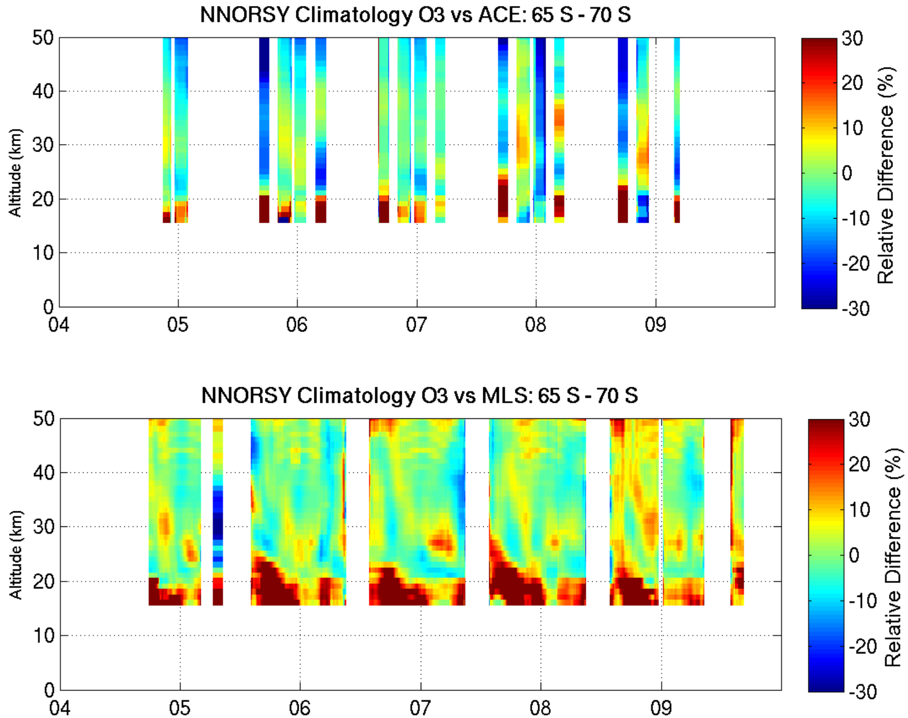

Fig. 11. Same as Fig. 8 but in the latitude band 65° S–70° S (Antarctic).

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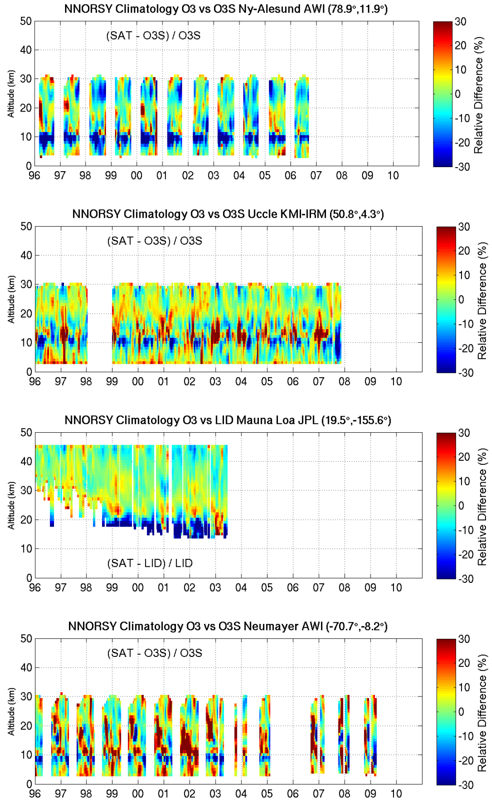

Fig. 12. Relative difference time series comparison of single stations for NNORSY climatology mode TLLO (SAT): Ny-Ålesund (Arctic), Uccle (northern mid-latitude), Nairobi (equator) and Neumayer (Antarctica). "O3S" denotes ozone sonde, "LID" ground-based lidar measurements. A one month running mean has been applied for the relative difference time series. For comparison of single measurements for these stations see Fig. 5.

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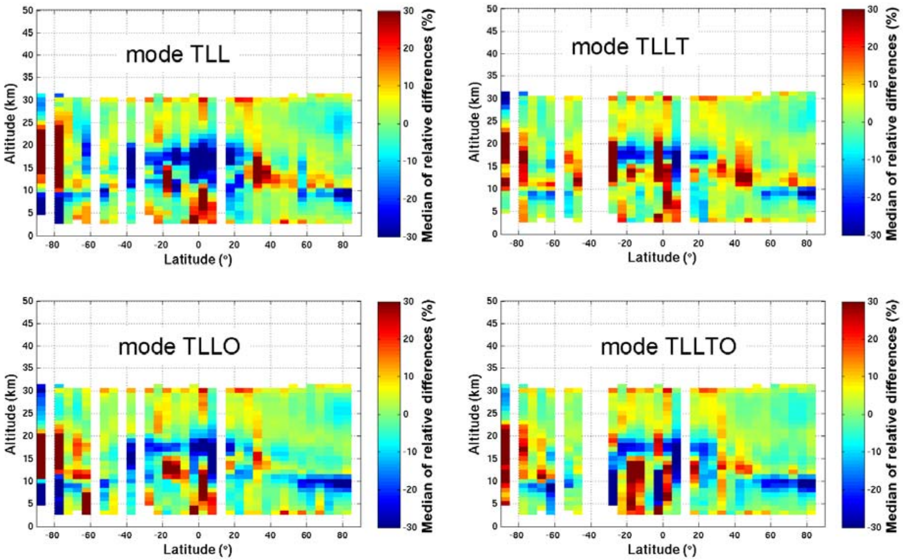

Fig. 13. Meridional structure of the median relative difference between NNORSY ozone profile climatology modes and GAW/NDACC/SHADOZ ozonesonde measurements.

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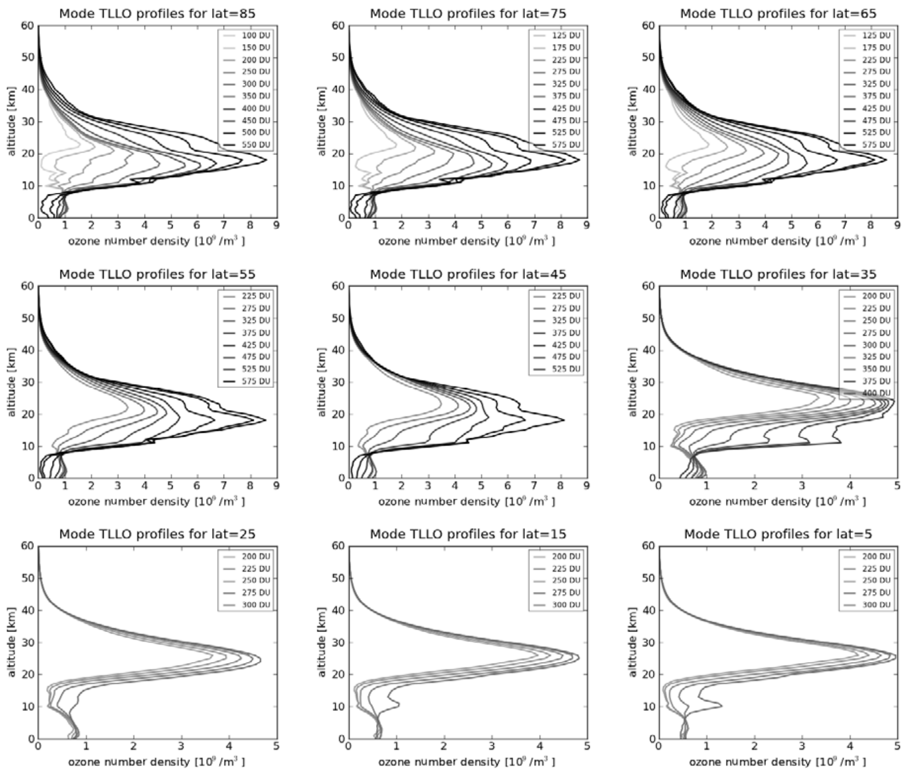

Fig. 14. Total ozone column dependency of mean NNORSY climatological ozone profile (mode TTLO) at different latitudes in the Northern Hemisphere.

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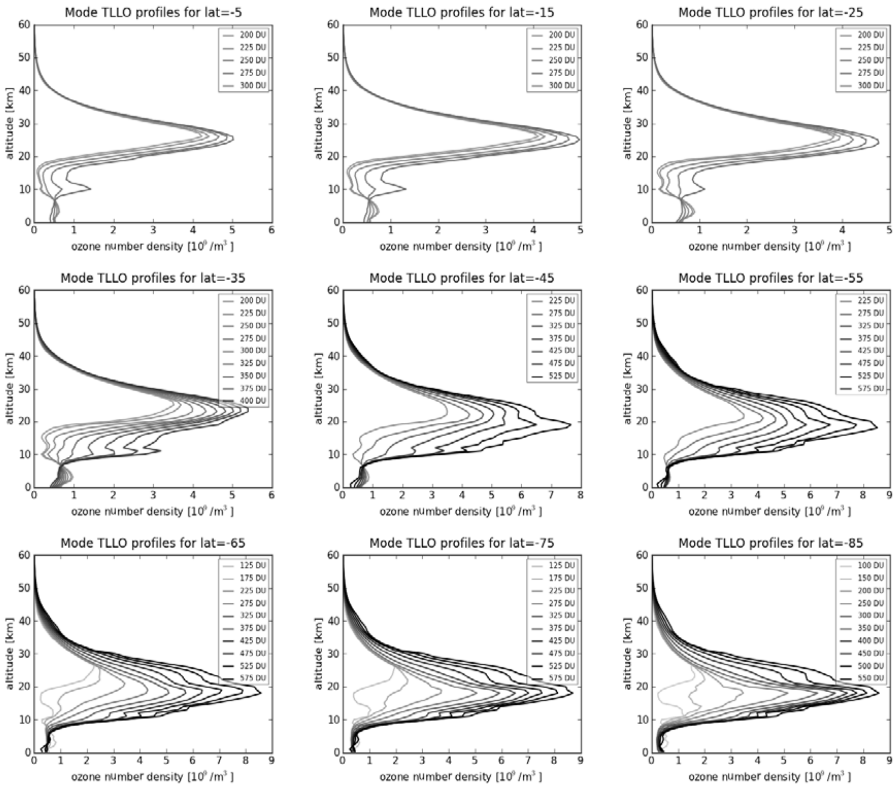

Fig. 15. Same as Fig. 13 but in the Southern Hemisphere.

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