Representation of ozone in the ECMWF model

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1 Introduction

Ozone is fully integrated into the ECMWF forecast model and analysis system as an additional three-dimensional model and analysis variable. The ECMWF ozone assimilation system (Hólm et al. 1999) allows the assimilation of ozone retrievals in form of ozone layers in 3D-VAR or 4D-VAR. Since April 2002, profiles from the SBUV/2 (Solar Backscatter Ultra Violet) instrument on NOAA-16 and total column ozone retrievals from GOME (Global Ozone Monitoring Experiment) on ERS-2 (provided by KNMI's Fast Delivery Service) have been assimilated in the operational ECMWF system. In the ECMWF 40-year re-analysis (ERA-40) project (Simmons and Gibson 2000), retrievals from TOMS and SBUV instruments on various satellites are assimilated in 3D-VAR with a horizontal truncation of T159 (about 125 km grid spacing) from December 1978 onwards.

2 Ozone model

The ECMWF forecast model includes a prognostic equation for the ozone mass mixing ratio O_3 $[kg/kg]$

$$\frac{dO_3}{dt} = R_{O_3} \tag{1}$$

where R_{O_3} is a parameterization of sources and sinks of ozone. Without such a source/sink parameterization the ozone distribution would drift to unrealistic values in integrations longer than a few weeks.

The parameterization used in the ECMWF model is an updated version of Cariolle and Déqué (1986), which has been used in the ARPEGE climate model at Météo-France. This parameterization assumes that chemical changes in ozone can be described by a linear relaxation towards a photochemical equilibrium. It is mainly a stratospheric parameterization. The relaxation rates and the equilibrium values have been determined from a photochemical model, including a representation of the heterogeneous ozone hole chemistry. The updated version of the parameterization (with coefficients provided by Pascal Simon, Météo-France) is

$$\begin{aligned} R_{O_3} \quad = \quad & c_0 + c_1(O_3 - \bar{O_3}) + c_2(T - \bar{T}) \\ & + c_3(O_3^{\uparrow} - \bar{O_3}^{\uparrow}) + c_4(Cl_{EQ})^2 O_3, \end{aligned} \tag{2}$$

where

$$O_3^{\uparrow}(p) = -\int_p^0 \frac{O_3(p')}{g} dp'. \tag{3}$$

Here c_i are the relaxation rates and $\bar{T}$, $\bar{O_3}$, and $\bar{O_3}^{\uparrow}$ are photochemical equilibrium values, all functions of latitude, pressure, and month. Cl_{EQ} is the equivalent chlorine content of the stratosphere for the actual year, and is the only parameter that varies from year to year. For the ECMWF model it was necessary to replace the photochemical equilibrium values for ozone with an ozone climatology (Fortuin and Langematz 1995) derived from observations. The heterogeneous term $c_4(Cl_{EQ})^2 O_3$ is only turned on below a threshold temperature of 195 K.

3 Ozone analysis

In the ECMWF analysis system there is no separate ozone analysis, but ozone is analysed simultaneously with all the other analysis variables in the 3D-VAR or 4D-VAR system. Ozone is analysed univariately at present, which means that the analysis increments of ozone and other variables are assumed to be uncorrelated. Ideally, we should take into account the correlation which exists between ozone increments and the dynamical increments and perform a multivariate analysis of ozone. However, in a multivariate analysis the ozone sensitive observations will directly change the dynamic analysis variables as well as the ozone field. Since a lot of the ozone observations (especially during the earlier years of ERA-40) are being assimilated for the first time in a dynamic model, it is not known if the quality of the data is good enough not to affect the atmospheric state adversely. To prevent ozone sensitive observations from directly changing any variable other than ozone, a univariate treatment was chosen.

For similar reasons, model ozone is not used directly in the radiation calculations of the forecast model, where the ozone climatology of Fortuin and Langematz (1995) is used instead. The only way ozone can affect the dynamics in 3D-VAR is through the use of the model ozone in the radiance observation operators. In the ECMWF model/analysis configuration this is a weak feedback, which should mostly improve the usage of radiance observations. In 4D-VAR ozone affects the dynamics through the adjoint integrations, even if the ozone analysis is univariate.

In the ECMWF assimilation system retrievals in the form of ozone layers or partial columns (unit kgm^{-2}) are assimilated, not ozone profile points. The main difficulty with the assimilation of retrieved ozone data, which are given as vertically integrated layers spanning several model levels (e.g. TOMS, GOME and SBUV retrievals), is how to distribute the analysis increments in the vertical. This distribution is controlled by the background error covariance matrix of the ECMWF assimilation system. The vertical covariances directly determine the weights with which the layer increment is spread in the vertical and hence the shape of the resulting analysis increment profile.

The ozone background error covariances used in the ECMWF system were determined statistically from an ensemble of analysis experiments. The observations used in each analysis were perturbed randomly according to the observation error. Differences between the background fields valid at the same time, but from different experiments are taken to be representative of the background error and give fields from which the background error statistics can be calculated (Anderson and Fisher, 2000).

4 Ozone observations

A comprehensive review of the availability and quality of ozone data from 1957 onwards can be found in the SPARC (1998) report on the assessment of trends in the vertical distribution of ozone. To be of use for the operational ECMWF analysis system, observations have to be available in near-real time (NRT), i.e. only a few hours after the observations are taken. Because of this requirement it was decided to use ozone retrievals from the GOME instrument on ERS-2 and from the SBUV/2 instrument on NOAA-16 in the operational system. The assimilation of ozone retrievals in the operational ECMWF model began on 9 April 2002. The GOME retrievals are the NRT total column data produced by KNMI's fast delivery service, version FD 3.1 (see http://www.knmi.nl/gome_fd/index.html for more information). The SBUV data come from NESDIS (see http://orbit-net.nesdis.noaa.gov/crad/sit/ozone/ for more information) and are combined at ECMWF into 6 ozone layers (0.1-1 hPa, 1-2 hPa, 2-4 hPa, 4-8 hPa, 8-16 hPa, 16 hPa-surface).

The data are currently used in the following way. SBUV data are not used at solar elevations less than 6°. GOME data are only used at solar elevations greater than 10° and between 40°N and 50°S. This 'conservative' approach was chosen because the bias between the GOME data and the model can be large outside this latitude band, and we wanted to minimize the impact of the ozone assimilation on the rest of the assimilation system, while the ozone analysis and the ozone chemistry are still undergoing tests and possible improvements. Variational quality control and first-guess checks are carried out for both data sets.

In the ERA-40 project, it was not necessary to have data available in NRT, and it was decided to assimilate total column ozone data from TOMS instruments and ozone layers from SBUV/2 instruments, which flew on various satellites from 1978 onwards. TOMS and SBUV data have been reprocessed for their whole recording period from 1978/9 onwards in an attempt to obtain a trend quality observation record, giving confidence that high quality data are used in ERA-40. The assimilation of ozone data into ERA-40 began in December 1978 and continued until August 2002. No ozone data were assimilated in 1989 and 1990 for technical reasons.

5 Validation of the ECMWF ozone field

5.1 Total ozone

To validate the ECMWF ozone analysis, analysed ozone fields are compared with independent observations, concentrating on ozone fields from ERA-40. Figure 1 shows a timeseries of monthly mean ERA-40 ozone values in Dobson Units (DU) and ground based total ozone from four stations for the whole ERA-40 period from 1957 to 2002. We see good agreement for those years when TOMS and SBUV data assimilated (1979-1988; 1991-2002, though with some gaps in coverage). There are some biases, e.g. the minima are not low enough at Barrow and Bismarck, and values are slightly too low at Mauna Loa. The ozone hole is not quite deep enough at the South Pole in October, but the trend to lower total ozone values at the South Pole during the 1980s is well captured.

For the pre-1979 period ERA-40 total ozone is also reasonable during much of the years, but some larger biases can be seen. Bismarck and Barrow have a good annual cycle in the years prior to 1972, when no satellite data of any sort are assimilated in ERA-40. Between 1972 and 1979 data from the Vertical Temperature Profiler Radiometer (VTPR) are assimilated into the ERA-40 system. Too high late-winter values are seen during those years (1972-1978) when no ozone data but VTPR data are assimilated. The same can be seen in 1989 and 1990, when no ozone data but TOVS-1b data are assimilated. This suggests that the assimilation of these satellite data might upset the Brewer-Dobson circulation, possibly either through a forcing due to the strong convection excited in the tropical troposphere due to the spin-up problem or through a forcing caused by correcting biases in the upper stratosphere. The effect of this on ozone is be masked when TOMS and SBUV data are assimilated. The timeseries for tropical station at Mauna Loa is very similar in the pre-1979 period to the later years.

The most noticeable difference between ERA-40 ozone and the ground based observations prior to 1979 is seen at the South Pole, where total ozone in ERA-40 is underestimated in many months. The low ERA-40 ozone values during southern spring are a result of the ozone chemistry parameterization. The equivalent chlorine loading, which determines the strength of the heterogeneous term in the chemistry parameterization (see Equation 2), is smaller during the earlier years of ERA-40 than in later years, but it is not zero. Comparisons with ozone sondes from Amundsen-Scott during the 1960s show that ERA-40 ozone values are considerably lower than sonde values below the ozone maximum. They also show that ERA-40 temperatures are about 30K lower than the sonde temperatures at Amundsen-Scott during October, and considerably below the temperature threshold for PSC formation. At these

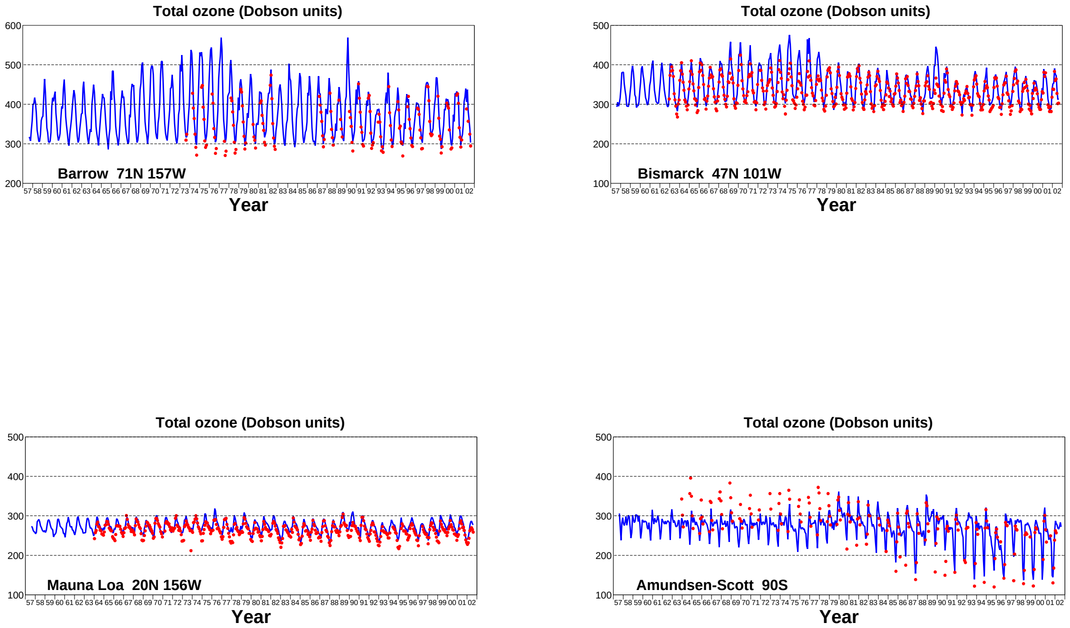

Figure 1: Timeseries of monthly mean total ozone in DU from ground based observations (red dots) and ERA-40 (blue curve) for the stations Barrow, Bismarck, Mauna Loa, and Amundsen-Scott. Figure provided by Adrian Simmons.

temperatures the heterogeneous term in Equation 2 is active and some of the ozone is depleted in an 'ozone hole like' manner in ERA-40 during these early years. During the rest of the year, the ozone maximum at the South Pole is located at higher altitude in ERA-40 than in the observations, and ozone values below the maximum are too low, resulting in a lower total column value. It is possible that the ozone climatology used in the ECMWF system is not appropriate for South Pole conditions during the early years.

During the later years of ERA-40, the PSC term in the ozone chemistry is not strong enough to produce a deep enough ozone hole if no ozone data are assimilated. This is illustrated in Figure 2. The top plots show the total ozone field in DU on 30 September 1990 from ERA-40 (no ozone observations were assimilated in 1989 and 1990). The middle plots show the total ozone field for the same day from an experiment which uses the ERA-40 configuration and in which TOMS and SBUV ozone observations are assimilated. The bottom plots show TOMS data for the same day. Note that while the analysed ozone fields are at 12z, TOMS needs 24 hours to cover the whole globe and the map shown is a daily composite. Even without the assimilation of ozone data, the model captures the main features seen in the TOMS data. Because the large scale ozone field is strongly determined by the atmospheric dynamics, and the wind analysis in the ECMWF system is good, the model captures the main features seen in the TOMS data even with the relatively simple chemistry parameterization. However, in areas where the chemistry is important the agreement is not so good. The Antarctic ozone hole is not deep enough if no ozone data are assimilated. Furthermore, a bias is apparent in the circum-antarctic ozone belt, where ozone values are too high in ERA-40. When ozone data are assimilated the ozone field is much improved.

The ECMWF total ozone field shows a bias relative to independent observations, that varies depending

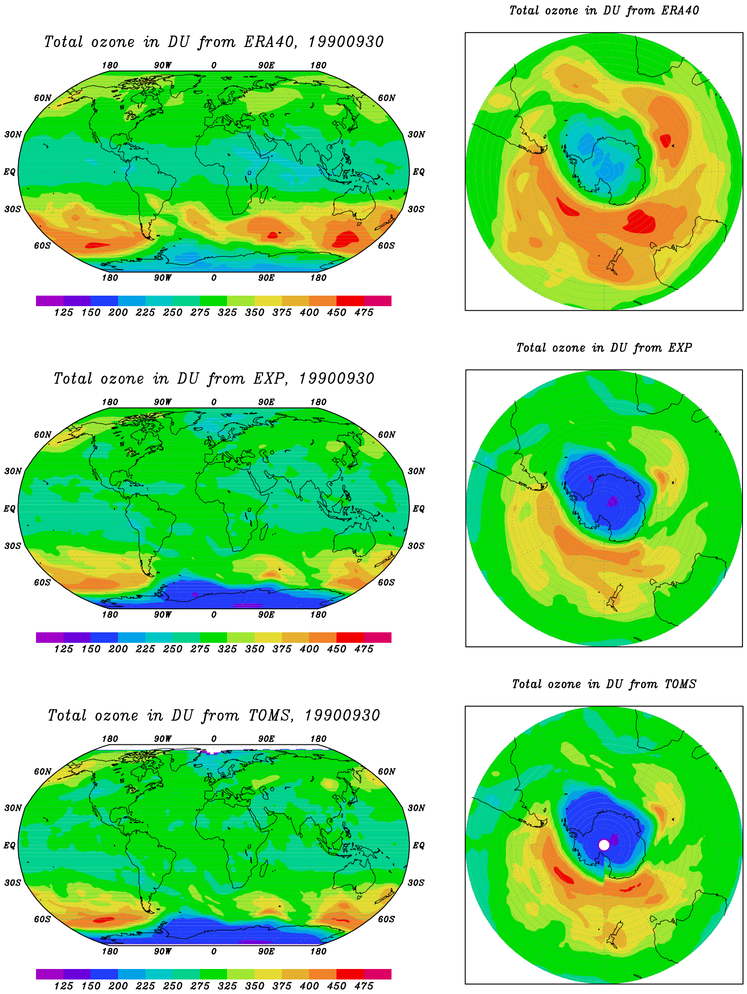

Figure 2: Total column ozone in DU on 30 September 1990 from the ERA-40 production in which no ozone observations are assimilated at this time (top), from an experiment which used the ERA-40 configuration and in which TOMS total column ozone and SBUV ozone layers are assimilated (middle), and from gridded daily TOMS data (bottom).

on the time of year and the geographical location. Generally, the model overestimates total column ozone in the extratropics and underestimates it in the tropics. The positive bias is largest at high latitudes in the NH during winter and spring. The reason for this model bias is not known at present. It is possible that the coefficients or the ozone climatology used in the ozone chemistry parameterization might not be appropriate for the ECMWF model. Alternatively, there are signs that the large scale vertical transport in the ECMWF analyses is too strong, so that the ozone bias could be a result of transport problems.

5.2 Midlatitude ozone profiles

To get an idea about the quality of the vertical distribution of analysed ozone field, ozone profiles from ERA-40 are compared with ozone sonde profiles from Hohenpeissenberg (47.8°N, 11°E), which were obtained from the WOUDC (World Ozone and UV radiation Data Centre). The ozone data are plotted in milli Pascal (mPa), which is proportional to the number density and allows one to compare the contributions from different layers to the total column in log pressure coordinates. Seasonal mean ozone profiles and standard deviations are calculated for JFM (January, February, March) and JJA

(June, July, August) for the years 1967-1971, 1973-1977, 1983-1987, and 1992-1995. A simple quality check is carried out for the sondes, and sondes that do not reach 40 hPa are discarded. The ERA-40 ozone profiles are the analysis profiles from the grid point closest to the sonde location and from the closest analysis time.

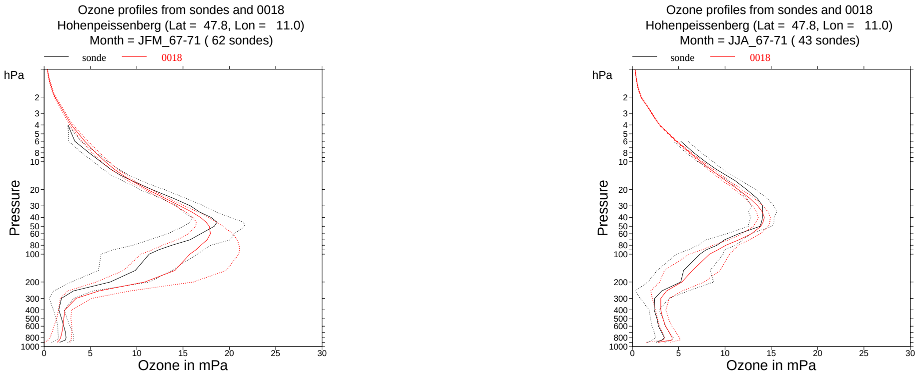

Figure 3: Mean ozone profiles in mPa at Hohenpeissenberg from sondes (black curves) and ERA-40 (red curves) for JFM (left) and JJA (right) 1967-1971. The solid line is the mean profile, the dotted lines +/- one standard deviation.

The ozone profiles for JFM and JJA 1967-1971 are depicted in Figure 3. During these years no satellite data are assimilated into ERA-40. Even without the assimilation of any ozone data, the JJA profiles agree well with the sondes, giving confidence that the model produces a reasonable ozone distribution in midlatitudes, even with a relatively simple chemistry parameterization. The agreement between the analysed profiles and the sondes in JFM is less good than in JJA. The ERA-40 ozone maximum is located at too low altitude, and the ozone values below the ozone maximum are too high. This corresponds to larger total column values in the analysis compared to observations, which is in agreement with the timeseries for the NH stations Barrow and Bismarck in Figure 1.

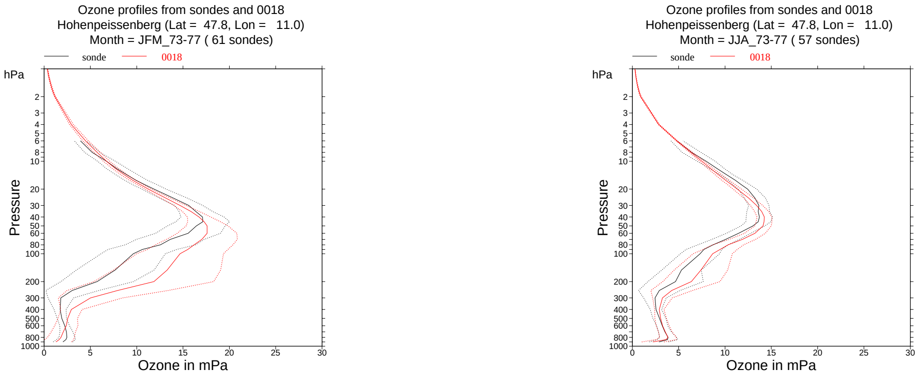

Figure 4: As Figure 3 but for 1973-1977.

Figure 4 shows the seasonal mean ozone profiles for the years 1973-1977 when no ozone data but VTPR data are assimilated. The differences betweeen ERA-40 profiles and sondes show the same behaviour as in Figure 3, but the deviations from the sonde profiles are larger, both during JFM and JJA. Again, this agrees with what is seen in the total column ozone plots (Figure 1), which show an increased bias at the NH stations for the years between 1972 and 1978.

While the assimilation of total column ozone data clearly improves the ECMWF total ozone field, a bias between the model and the data can lead to problems in the vertical distribution of ozone in the analysis. Problems arise from having to distribute large total column analysis increment in the vertical.

The way the analysis increments are distributed in the vertical is determined by the background error covariance matrix of the ECMWF analysis system. The covariances for ozone originally used in the ECMWF system (and used in ERA-40 from 1991 to October 1996) had anti-correlations between the stratosphere and the troposphere. In situations where the analysis increments were large, the increments were distributed in the vertical in such a way that they can cause an almost complete depletion of ozone in the upper troposphere/ lower stratosphere and an overestimation of ozone in the lower troposphere (Dethof and Hólm 2002). This can be seen in JFM 1992-1995 (Figure 5), when TOMS data from NIMBUS-7 and SBUV/2 data from NOAA-11 are assimilated. During JJA, when the bias is smaller, the analysis ozone profiles are considerably better than during JFM.

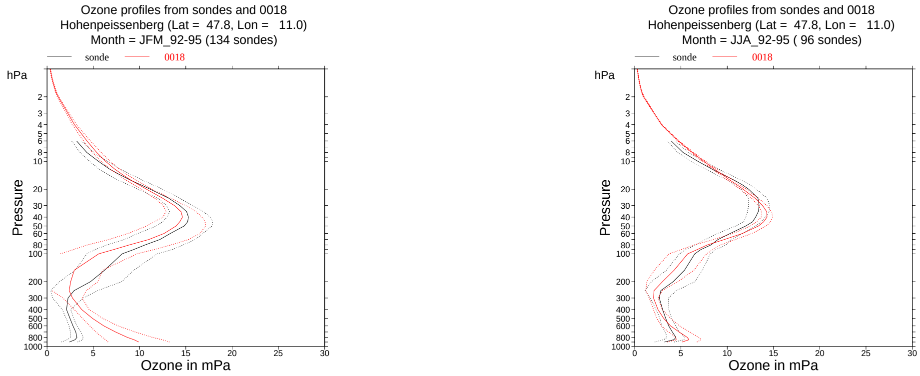

Figure 5: As Figure 3 but for 1992-1995.

When this problem was noticed, the ozone covariances were modified, and the anti-correlations between the stratosphere and the troposphere removed. The modified covariances are currently used in the operational system, and were used in ERA-40 between October 1996 and August 2002, and also from the beginning of the ozone assimilation in December 1978 until 1989. With the new covariances the analysis increments are more confined in the vertical, and there are no anti-correlations between the stratosphere and the troposphere, or between levels at and above the stratospheric ozone maximum. However, while this improves the profiles in the troposphere and lower stratosphere, the ozone maximum can be reduced too much in situations where the analysis increment is large and negative. This can be seen in the JFM profiles for 1983-1987 (Figure 6) when TOMS and SBUV data from NIMBUS-7 are assimilated. The ERA-40 ozone maximum values in JFM are considerably lower than the sonde maximum. The JJA profiles agree well with the sondes.

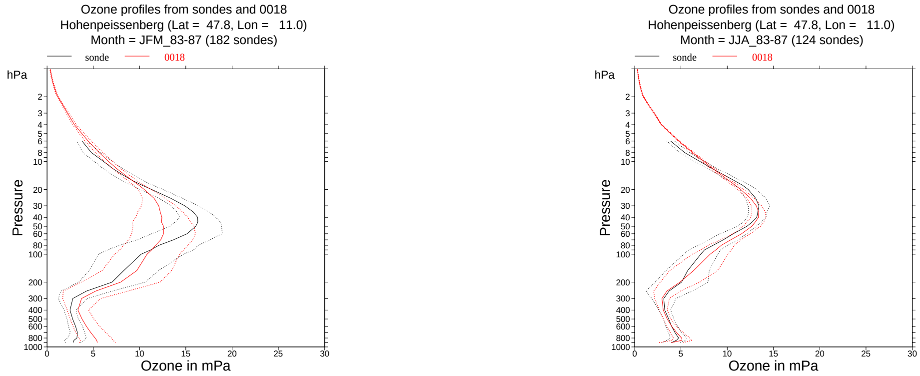

Figure 6: As Figure 3 but for 1983-1987.

The comparisons of ERA-40 profiles with ozone sondes highlight some problems with the vertical distribution of ozone in the NH during the winter months for years when ozone data are assimilated. Work is under way to improve the vertical structure of the analysed ozone field. Several aspects have to be considered here. First, a better representation of the ozone background error covariances is needed. Secondly, the bias between the data and the model has to be removed. This problem is two fold, because both the data and the model can have biases. Work is required to understand the reason for the model bias and how to reduce it. Biases in the data will be corrected by implementing a bias correction scheme for ozone data, which makes use of independent ground based observations to correct biases in the data.

6 Bias correction for ozone data

A simple bias correction scheme for total column ozone data has been developed to address some of the problems discussed in the previous section. This scheme makes use of independent ground based observations from Brewer or Dobson instruments, which are available from the WOUDC. The impact of the bias correction scheme on the analysed ozone field is illustrated for GOME total ozone data from KNMI's fast delivery service. The KNMI data have a bias compared to ground based observations. This bias shows a linear dependence on solar zenith angle. The GOME data are lower than independent observations at high solar zenith angles and higher at low solar zenith angles. A simple linear regression gives

$$OBS_{bc} = [1 - (3.5 - .1 * SZA)/100] * OBS, \tag{4}$$

where OBS is the value of the total column observation in DU, SZA the solar zenith angle, and OBS_{bc} the bias corrected value.

Assimilation experiments have shown that applying the bias correction to GOME data improves the fit of the observations to the analysis. Assimilating the bias corrected data also leads to improved vertical ozone profiles. An example is shown in Figure 7. Three assimilation experiments are started on 1 October 2002. In Exp-A no ozone data, in Exp-B the bias corrected GOME data, and in Exp-C the uncorrected GOME data are assimilated. Figure 7 compares an ozone sonde profile from Ny-Aalesund on 11 October 2002 with profiles from the three assimilation experiments. The ozone profile from Exp-A fits the sonde well at and below the ozone maximum, but values are slightly too high above the ozone maximum. At this time of year the model's ozone field is reasonable in the NH, and hence the model profile fits the ozone sonde well even without the assimilation of ozone data. The profile from Exp-C shows the same problems as seen in Figure 6. The ozone values at the maximum are reduced too much, and agreement with the sonde is worse than in Exp-A. Assimilating the bias corrected data (Exp-B) improves the fit to the sonde above the ozone maximum, while the ozone maximum is hardly changed compared to Exp-C.

These first results are encouraging and show the benefit of applying a bias correction to ozone data before assimilating them. It is planned to implement the bias correction scheme for total column data in the operational model after further testing. This bias correction scheme does not address the problems caused by the model bias. Additional work is required to understand the reason for the model bias and how to reduce it.

7 Summary and Outlook

With its relatively simple ozone chemistry parameterization the ECMWF model manages to reproduce a realistic ozone field in many situations. However, there are some biases compared to independent

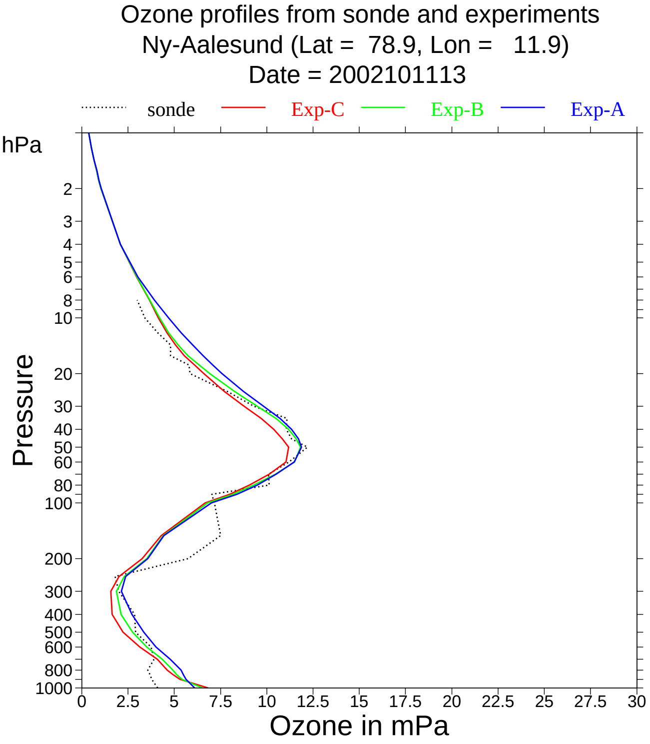

Figure 7: Ozone profiles in mPa at Ny-Aalesund on 11 October 2002 from sonde (black), Exp-A (blue), Exp-B (green) and Exp-C (red).

observations. For example, total ozone values at high latitudes in the NH during winter and spring are too high, and the very low ozone values observed in the Antarctic ozone hole are not reproduced well.

Ozone retrievals from various TOMS and SBUV instruments are assimilated in the ERA-40 analysis system, and retrievals from GOME and SBUV/2 are assimilated in the operational ECMWF model. The assimilation of ozone data leads to a good total column ozone field in the ECMWF analysis that agrees well with observations. However, additional work is required to improve the vertical distribution of ozone in the analyses. This work includes an improvement of background error covariances for ozone, and it also has to address the problems of a bias between observations and the model. Work to develop a bias correction scheme for ozone data has already started, and the problem of a model bias will be addressed in the near future.

Preparations are underway to make use of new satellite data that give more information about ozone in the stratosphere. NRT retrievals from various instruments onboard ESA's ENVISAT are currently monitored at ECMWF. These data include retrievals from MIPAS and GOMOS that give information information about ozone (and temperature and water vapour) in the stratosphere and mesosphere at a better vertical resolution than the ozone data currently used at ECMWF. In addition, SCIAMACHY gives total column ozone data, which could be an alternative to the ozone data from GOME. Once the quality of the ENVISAT data is established and the data products are stable, the active assimilation of the data will be tested.

Acknowledgements

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