Ozone in ERA-40: 1991-1996

A. Dethof and E. Hólm

European Centre for Medium-Range Weather Forecasts

1 Introduction

Ozone is a prognostic variable in the ECMWF model and is included in the analysis system in a univariate way.The ozone analysis is included in the ECMWF 40-year re-analysis project plan (ERA-40) (Simmons and Gibson, 2000) for years when ozone observations are available. TOMS (Total Ozone Mapping Spectrometer) total column ozone retrievals and SBUV (Solar Backscatter UltraViolet) layer ozone retrievals from various platforms are assimilated in ERA-40.

In this workshop paper we only give a short discussion of the ozone analysis in ERA-40. A more detailed discussion can be found in Dethof and Hólm (2002).

2 Ozone chemistry

Ozone is fully integrated into the ECMWF forecast model and analysis system as an additional three-dimensional model and analysis variable similar to humidity. The 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 source/sink parameterization must maintain a realistic ozone distribution over several years of integration, without reducing the dynamic variability of ozone. In addition, we would like the parameterization to be able to create an Antarctic ozone hole when the conditions are right.

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

$$\begin{aligned} R_{O_3} &= c_0 + c_1(O_3 - \bar{O}_3) + c_2(T - \bar{T}) \\ &\quad + c_3(O_3^{\uparrow} - \bar{O}_3{}^{\uparrow}) + c_4(Cl_{EQ})^2 O_3, \end{aligned} \tag{2}$$

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 ozone parameterization is only active in daylight, and the heterogeneous part is only turned on below a threshold temperature of 195 K.

3 Ozone analysis

In the ERA-40 system there is no separate ozone analysis, but ozone is analyzed simultaneously with all the other analysis variables in the 3D-VAR system, and ozone sensitive observations are treated just like any other observation. In the 3D-VAR system, ozone is analyzed univariately, 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 3D-VAR analysis the ozone sensitive observations will directly change the dynamic analysis variables as well as the ozone field. Since most of the ERA-40 ozone observations 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 is 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 is through the use of the model ozone in the radiance observation operators. In the ERA-40 model/analysis configuration this is a weak feedback, which should mostly improve the usage of radiance observations.

4 Validation of the ozone field in ERA-40

4.1 Total column ozone

Even without the assimilation of ozone data the ECMWF model produces a realistic and stable ozone field, which is in broad agreement with gridded daily TOMS data. The top colour plot of Figure 1 shows the total column ozone field in Dobson Units (DU) on 10 February 1992 from a model run, which is started on 1 December 1991 and in which no ozone observations are assimilated. The bottom plot shows the TOMS data for the same day. Note that while the ozone field from ERA-40 is at 12z, TOMS needs 24 hours to cover the whole globe and the map shown is a daily composite.

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. The zonal mean relative differences between the fields are less than 10 % over large parts of the globe. Compared to the TOMS data, the model underestimates total column ozone in the tropics and overestimates it at high latitudes.

The middle colour plot of Figure 1 shows the analyzed total column ozone field in DU on the same day from the ERA-40 production, in which TOMS total column ozone data and SBUV ozone layers are assimilated. The figure clearly shows that the analysis is drawing to the data and that the agreement between the analysis and the observations is very good. The zonal mean relative differences between the analyzed field and the TOMS data are now less than 2% everywhere.

Figure 2 shows the timeseries of zonal mean total column ozone in DU from 1991 to the end of 1996 from ERA-40 and TOMS data. From 1991 onwards, TOMS and SBUV data from various platforms are assimilated in the ERA-40 system. The differences between the analyzed ozone field and the TOMS data are small, and the analyzed field reproduces well the seasonal variations seen in the TOMS data, as well as the inter-annual variability. For instance, lower total column ozone values are observed over large parts of the globe during the years following the eruption of Mt. Pinatubo (15 June 1991). This decrease in total column ozone is seen in the analyzed ozone field, for example the lower total column values at high northern latitudes and in the circum-antarctic ozone maximum in 1992. The Antarctic ozone hole is also well captured in the ozone analysis. Note that TOMS data from several instruments were assimilated between 1991 and 1996 and that there are periods when no TOMS data were available.

4.2 Stratospheric ozone

A zonal mean cross section of the analyzed stratospheric ozone and of ozone from SBUV in ppmm (parts per million mass) are plotted in Figure 3 for 3 January 1994. The figure shows that the large scale zonal mean structure of the analyzed ozone in the stratosphere is reasonable. We can see that the gradient between the low tropospheric ozone values and the higher stratospheric values is well captured in ERA-40, as is the location of the tropical ozone maximum. However, the maximum values of the SBUV data in the tropics are generally slightly higher than the analyzed values.

To further evaluate the quality of the ozone field in ERA-40, the analyzed fields are compared with independent ozone sonde observations, which are not used in the analysis. Figure 4 shows ozone profiles from ERA-40 and from ozone sondes at Ny-Aalesund for January 1996. The ozone sondes were obtained from the Network for the Detection of Stratospheric Change (http://www.ndsc.ncep.noaa.gov/). The profiles illustrate that there is a problem with the vertical structure of the ozone field in ERA-40. The ozone maximum is overestimated in the analysis, around the tropopause level ozone concentrations are much too low, and near the surface ozone values are too high. This problem is particularly pronounced at high latitudes during winter and spring. It suggests that while the analyzed total column values are good, there are problems with the distribution of the analysis increments in the vertical, particularly in the troposphere and at high latitudes.

The distribution of the analysis increment in the vertical is the main difficulty with the assimilation of the TOMS and SBUV retrieved ozone data, which are given as vertically integrated layers spanning several model levels. It is controlled by the background error covariance matrix of the ECMWF 3D-VAR assimilation system. The vertical correlation matrix for ozone used before October 1996 had anti-correlations between the stratosphere and the troposphere. In situations where the total column analysis increments were large these anti-correlations led to an overestimation of ozone near the surface, a strong reduction of ozone in the upper troposphere and an overestimation of the stratospheric ozone maximum (as seen in Figure 4).

On the basis of single observation experiments, new covariances were designed and implemented on 25 October 1996. These covariances do not have the anti-correlations between the stratosphere and troposphere and the resulting analysis increment is more confined in the vertical. However, with the new background errors for ozone there are still problems in situations where the analysis increment is large, for example at high northern latitudes in winter, when the model has a positive bias compared to TOMS data. In these situations the ozone maximum in the analyzed profiles is much reduced compared to observations. The fact that problems with the vertical distribution of ozone remain, highlights the need to replace the static observation errors for ozone by flow dependent ones, which take into account the local values of ozone when assigning the background errors. The static background errors are global averages, which mostly reflect the tropics. Regions where the background ozone values are much different from the tropics are still found to have problems with the vertical distribution of ozone increments even after the stratosphere-troposphere anti-correlations have been removed. Users of the ERA-40 data should be aware that there can be problems with the vertical structure of the analyzed ozone field.

5 Conclusions

Ozone retrievals from various TOMS and SBUV instruments are assimilated in ERA-40 between 1991 and 1996. The resulting total column ozone field is generally good and agrees well with observations. The analyzed stratospheric ozone is also good over large parts of the stratosphere. However, there can be problems with the vertical structure of the analyzed ozone field, particularly in the troposphere at high latitudes in winter and spring. These problems come from the vertical correlation matrix used for ozone and illustrate the need to replace the globally averaged, static background errors for ozone by flow dependent ones, which take the local values of ozone into account when assigning background errors. Such flow-dependent covariances are currently being developed and will replace the current covariances in possible ERA-40 reruns.

A final word of advice. When comparing the analyzed ozone field from different years it should be kept in mind that data from different satellites are assimilated between 1991 and 1996, and that there are periods when no data are assimilated or periods when no TOMS data are available.

References

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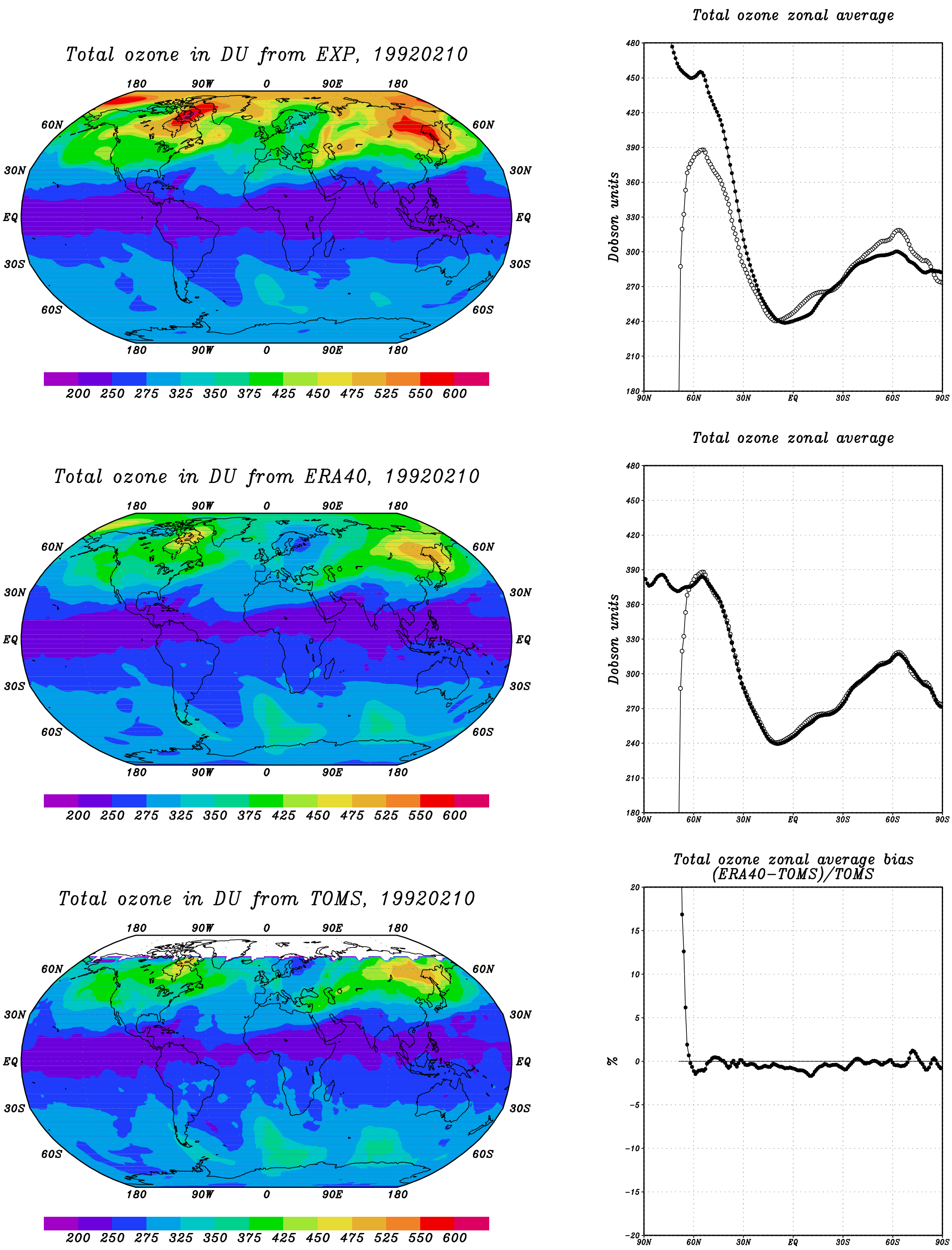

Figure 1: Colour plots: Total column ozone in DU on 10 February 1992 from a model run in which no ozone observations are assimilated (top), from the ERA-40 production in which TOMS total column ozone and SBUV ozone layers are assimilated (middle), and from gridded daily TOMS data (bottom). The top and the middle plot on the right show the zonal average total ozone values from the model (dark curve) and from the TOMS data (open circles). The bottom plot on the right shows the relative zonal mean difference between ERA-40 and the observations in %.

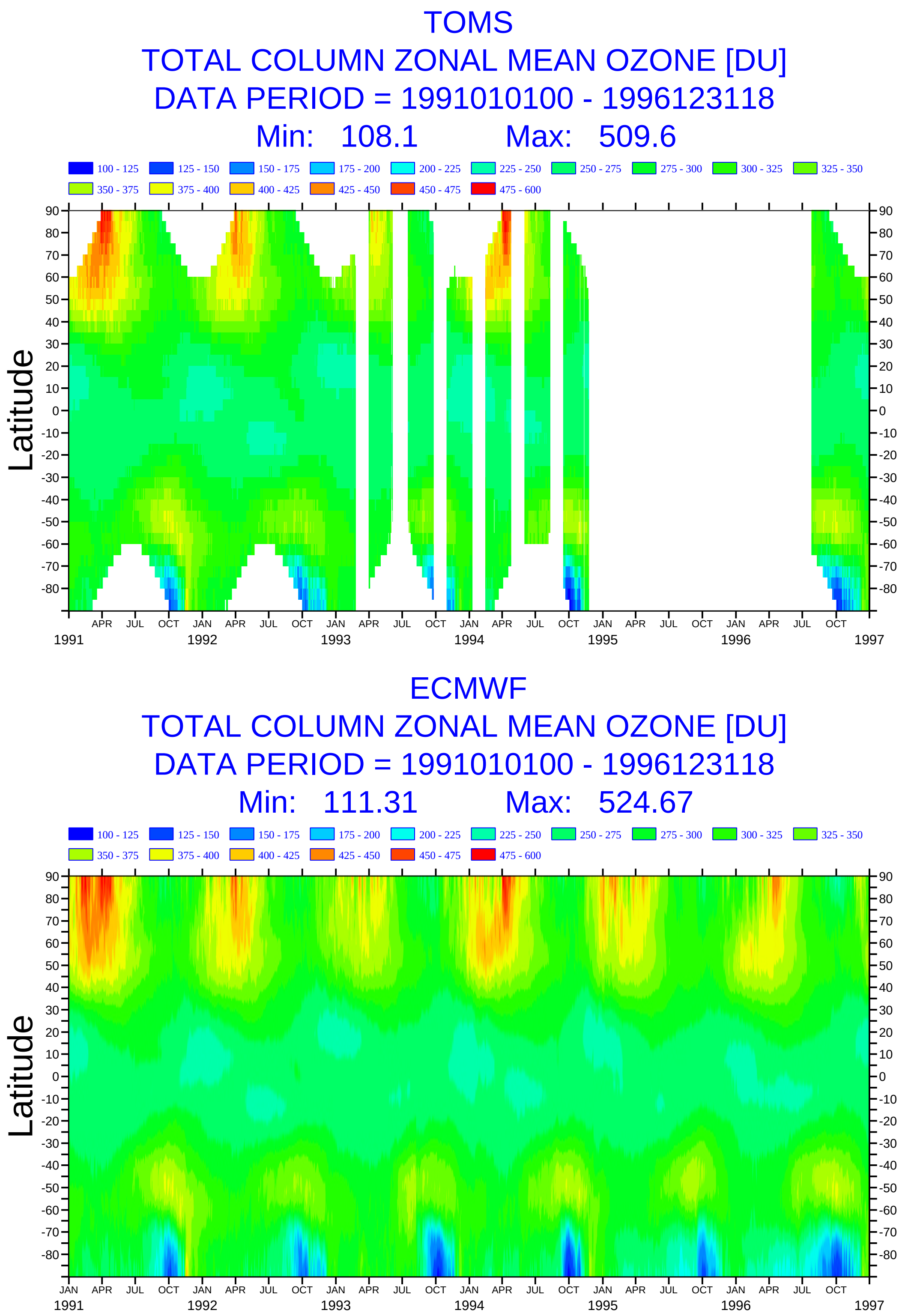

Figure 2: Time series of zonally averaged total column ozone in DU from 1991 to the end of 1996 from TOMS data (top) and ERA-40 (bottom).

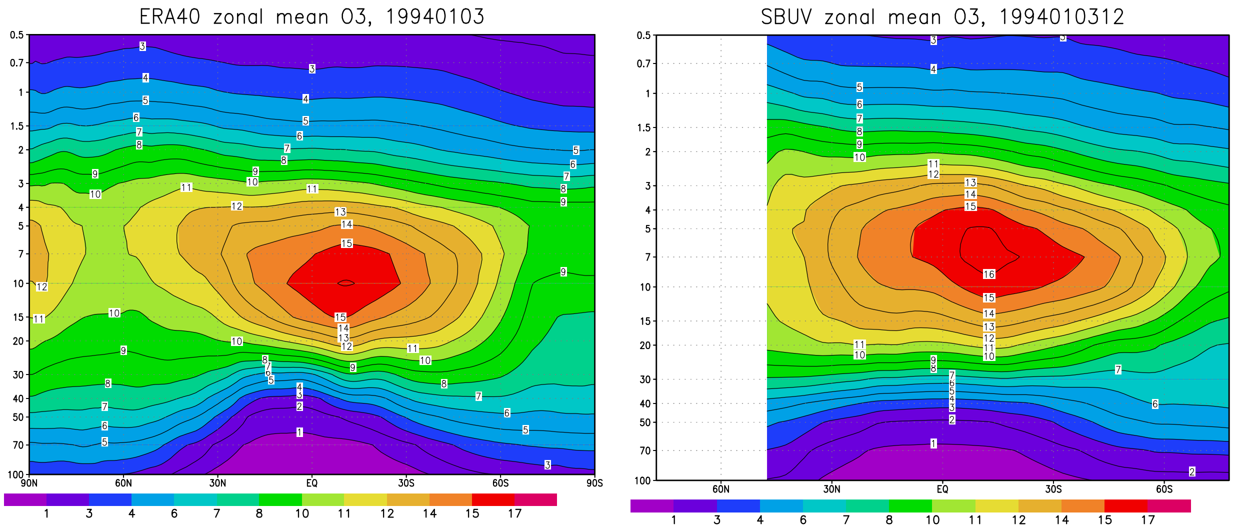

Figure 3: Vertical cross section of zonal mean ozone in ppmm on 3 January 1994 from ERA-40 (left) and SBUV (right).

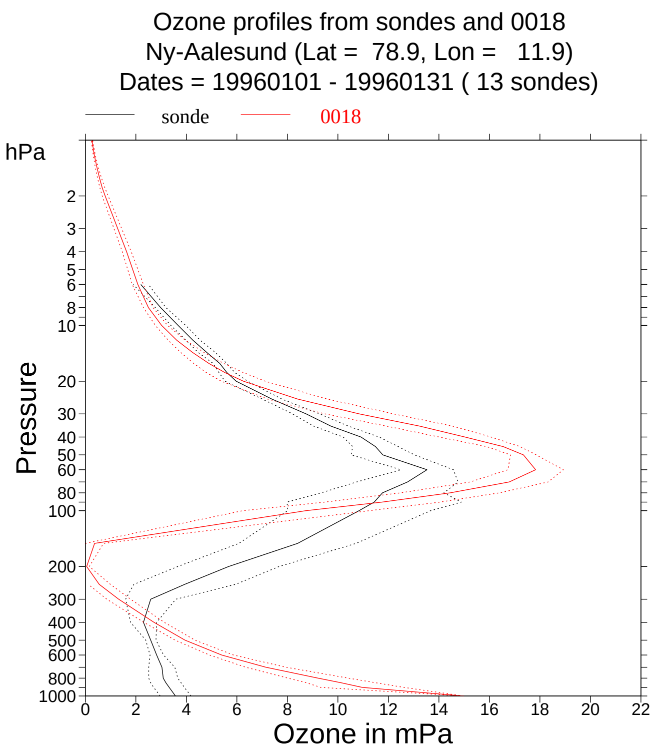

Figure 4: Ozone profiles in mPa at Ny-Aalesund from sondes (black curves) and ERA-40 (red curves) for January 1996. The solid line is the mean profile, the dotted lines +/- one standard deviation.