SHORT RANGE SIMULATIONS OF EXTRATROPICAL TOTAL OZONE WITH ARPEGE/IFS

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Abstract

This paper presents short range simulations with the climate version of ARPEGE of the evolution of total ozone in the Northern Hemisphere extratropics during a short period of the 1991-92 EASOE stratospheric measurement campaign. In the atmospheric regions and in the season of interest here ozone is to a good approximation a passive tracer in both the real atmosphere and in the model runs, and the errors in the simulated ozone fields are thus mainly determined by errors in the initial ozone distribution and errors in the subsequent evolution of the model dynamics. The relationship between errors in geopotential heights and errors in total ozone is discussed with the aim of examining the potential benefits of including ozone as an advected quantity in numerical weather prediction models.

INTRODUCTION

Short to medium range simulations of the stratospheric ozone concentration field is an area that has attracted an increasing amount of interest in recent years. A major reason for this is the concern about the possible anthropogenic depletion of the ozone layer and the biological hazards associated herewith. Considerable efforts have gone into both chemical and dynamical modelling work as well as into ground-based and satellite-based measurements. As a result of this we now have a fair amount of knowledge of the dynamical and chemical processes that are important for the tendency in ozone mixing ratios at different times and places in the atmosphere. This also means that ozone - with the possible exception of water vapour - is by now the most thoroughly studied and measured atmospheric trace gas that exists.

Although ozone chemistry is complicated and involves on the order of 50-60 different trace species, several model studies have shown that the evolution of total ozone outside the tropical regions can be simulated quite well up to one week ahead in time by letting a general circulation model advect the ozone, starting from a known ozone distribution at the initial model time (Riishøjgaard et al., 1992; Orsolini et al., 1993). In both of these studies photochemical sources and sinks for ozone were taken into account by means of a simple parameterisation scheme. That this kind of short range ozone simulations are possible is readily understandable also from a more theoretical point of view, as the variability on this time scale is mainly controlled by the dynamics in the lower stratosphere where the photochemical lifetime of ozone is on the order of months (Brasseur and Solomon, 1986).

Ozone production occurs mainly in the middle and upper tropical stratosphere, while ozone destruction normally takes place near the ground. In recent years destruction of ozone molecules has been shown also to take place in the springtime polar lower stratosphere (see e.g. Solomon, 1990), where the atmospheric chlorine normally fixed in reservoir compounds can be 'activated' through heterogeneous processes taking place on the surface of polar stratospheric cloud (PSC) particles. The active chlorine compounds can thus take part in a series of catalytic reactions, the net result of which is the destruction of ozone molecules. Strictly speaking the occurrence of these processes means that the approximation that ozone is a passive tracer in the extratropical lower stratosphere is no longer valid. However, the regions in which they take place are limited in space and time, and model studies indicate that the rates at which these reactions can destroy ozone is at most 1.5 DU (Dobson Units) per day, or on the order af 0.5%, and we can thus ignore the effects of them for short range simulations (Chipperfield et al., 1993).

In the middle and upper stratosphere the ozone mixing ratio is a tracer quantity in the winter hemisphere, while it is close to the photochemical equilibrium in the tropics and in the summer hemisphere. The change in equilibrium concentration takes place on a seasonal timescale, and as also the advective timescale is long at these altitudes we do not introduce any serious errors in short range ozone simulations by assuming that ozone everywhere outside of the tropics is a passively advected quantity.

In the following we will present a series of 10 day general circulation model simulations of the evolution in the stratospheric ozone field during the 1992-92 EASOE measurement campaign. We will present various methods for calculating the three-dimensional ozone distribution needed at the initial model time, and we will discuss the forecast errors in both dynamics and in total ozone. Finally we will discuss the contributions to the error in the ozone forecast from the initial ozone field and from the error in the evolution of the model dynamics.

THE MODEL AND THE INITIAL OZONE FIELD

We use the METEO-FRANCE climate version 0 of the ARPEGE/IFS global spectral model (for a detailed description see Déqué et al., 1993). In this configuration the model has 30 vertical levels, with about 10 in the troposphere, 17 in the stratosphere, and the remaing three in the mesosphere. In addition to all the physical parameterisation routines commonly found in GCMs the ARPEGE features ozone as a predicted variable. There is an ozone advection equation, and sources and sinks are parameterised on model variables using the method described by Cariolle and Déqué (1986). The model has been extensively validated both in long-term AMIP type runs (Déqué et al., op. cit.) and in short term simulations similar to the ones described here (Orsolini et al., 1993).

We run the model at truncation T42, and the starting points of the simulations are January 16, 1992, 12 Z, and January 22, 1992, 12 Z. We use ECMWF analysis fields for model initialisation up to the top analysis level at 10 hPa, and above this level we use climatological fields. Each experiment is run for 10 model days.

As ozone is a passive tracer the determination of the three-dimensional distribution of ozone mixing ratios at the initial model time is crucial for the quality of the subsequent ozone forecast. The vertically integrated ozone column is routinely measured from satellites, but as the number of vertical ozone soundings is very limited, one has to devise an initialisation scheme that generates a three-dimensional field from the two-dimensional total ozone field from the satellites, together with whatever other relevant information that is available.

An early attempt of doing so was described by Riishøjgaard et al. (1992; in the following referred to as R92). The idea was to use a simple analytical expression for the vertical ozone profile, namely the one used in the ECMWF forecast model

$$\int_0^p R_{O3} dp = \frac{a}{1 + \frac{b}{p}^{3/2}} \qquad (1)$$

where the integral of the mixing ratio, R_{O3}, from the top of the atmosphere down to a given pressure level, p, is expressed in terms of the two parameters, a and b. In the ECMWF forecast model a and b vary with longitude, latitude, and season, so as to give a good fit to the observed ozone climatology. R92 presented a parameterisation of a and b on model variables and on observed total ozone with the somewhat different aim of getting a good three-dimensional fit to an actual instantaneous ozone field. The R92 scheme has later been modified by Orsolini et al. (1993), who attempted to correct the missing downward displacement in ozone profiles inside the polar vortex of the R92-scheme.

It is an observational fact that ozone mixing ratios and potential vorticity are highly correlated on isentropic surfaces in the lower stratosphere. This was first pointed out by Danielsen et al. (1968), and has since been explored further by e.g. Vaughan and Price (1991), and Allaart et al. (1993). A simple and appealing idea is to use this relationship in reconstructing tracer fields. All available observations of PV, potential temperature, and ozone mixing ratios over a given interval of time can be put together to define a mapping from PV/θ-space to R_{O3}-space. This mapping can then be used for generating a tracer field from a meteorological analysis field alone at any time within the period for which the mapping is valid and at which an analysis is available. A scheme based on this principle was presented by Lait et al. (1990), and later a comprehensive scheme using the slightly different concept of "Equivalent PV Latitude" has been developed by Lary et al. (1993; in the following referred to as L93). The equivalent PV latitude (EPVL)of a given point on the globe is defined to be that of which the corresponding latitude circle encloses the same area as the PV-contour on which the point is found. It is thus essentially a normalized PV, in the sense that its horizontal integral remains unchanged whatever the meteorological conditions. In the simulations presented here we use the L93 initialisation and the method will be described briefly in the following section.

THE EXPERIMENTS

In order to have as large a set of vertical ozone soundings as possible available for generating the EPVL/θ- to R_{O3}- mapping we have chosen to do our experiments in connection with the EASOE measurement campaign of 1991-92. All available ozone measurements from the EASOE soundings from January 1 through January 9 of 1992 were binned in EPVL/θ- space by taking the PV values from the ECMWF analysis fields closest in time to each of the soundings, and this binning was used to define the mapping. Where data were missing (mainly for low PV values in the tropical and subtropical regions, and for high potential temperatures

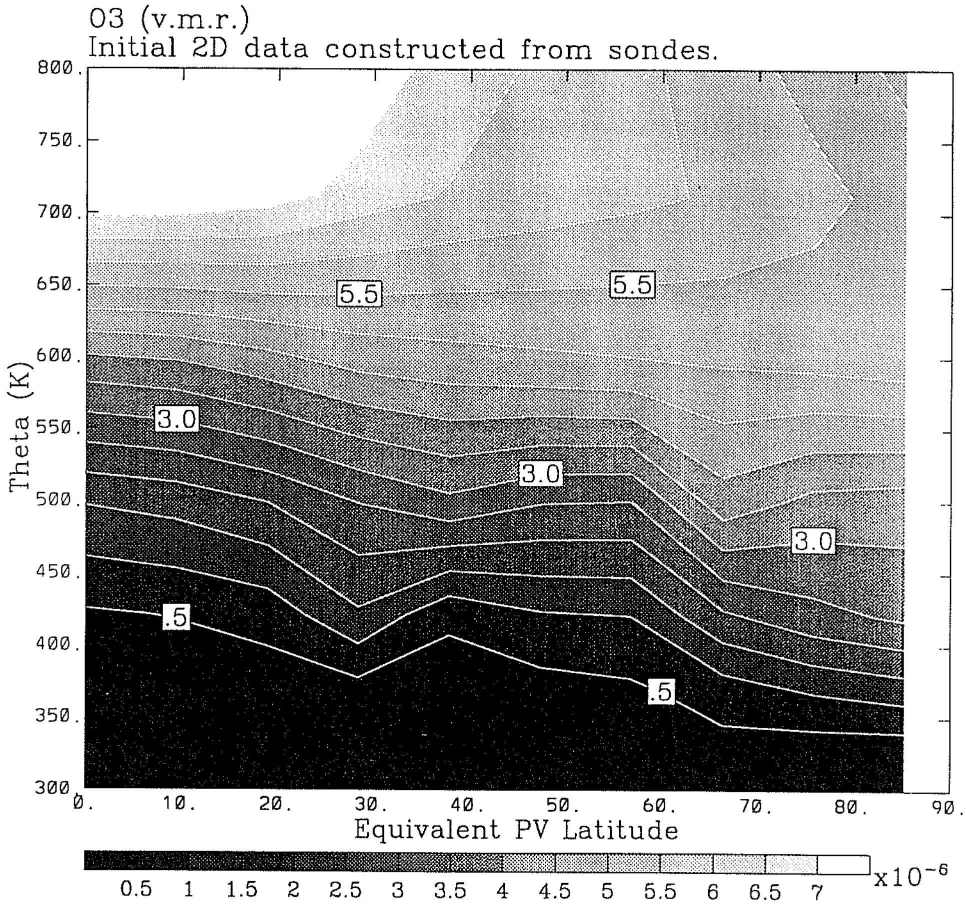


Figure 1 Mapping of EPVL/θ-space on to R_O3-space as defined by EASOE balloon soundings and ECMWF analysis fields. Where no data were available photochemical model values were used.

above the burst height of the sounding balloons) data of a two-dimensional photochemical model (Harwood and Pyle, 1980) were inserted together with climatological θ-values and geographical latitudes. The resulting mapping is shown in figure 1. Above the top analysis level at 10 hPa the ozone mixing ratio was assumed to be constant. Two sets of simulations were run, one starting on January 16, 12 Z, the other one on January 22, 12 Z. Figure 2a shows the vertical integral of the ozone field for January 16, 12 Z, as produced by the L93 initialisation, ie. when one applies the mapping shown in figure 1 to the EPVL- and θ-fields calculated from the ECMWF analysis of January 16, 12 Z. For comparison total ozone as measured by the TOMS instrument is shown in figure 2b. As the TOMS instrument is flown on a sun-synchroneous polar orbiter the measurements are asynoptic. A simple correction for this, consisting of doing a linear interpolation in time between two successive TOMS measurements, was carried out both for the initial times and for the validation times.

The large scale factures are clearly seen to be well captured: There is a large minimum centered over Western Europe, and major maxima centered over the eastern part of the USA, and over Eastern Siberia, respectively. The latter maximum is separated from a minor one

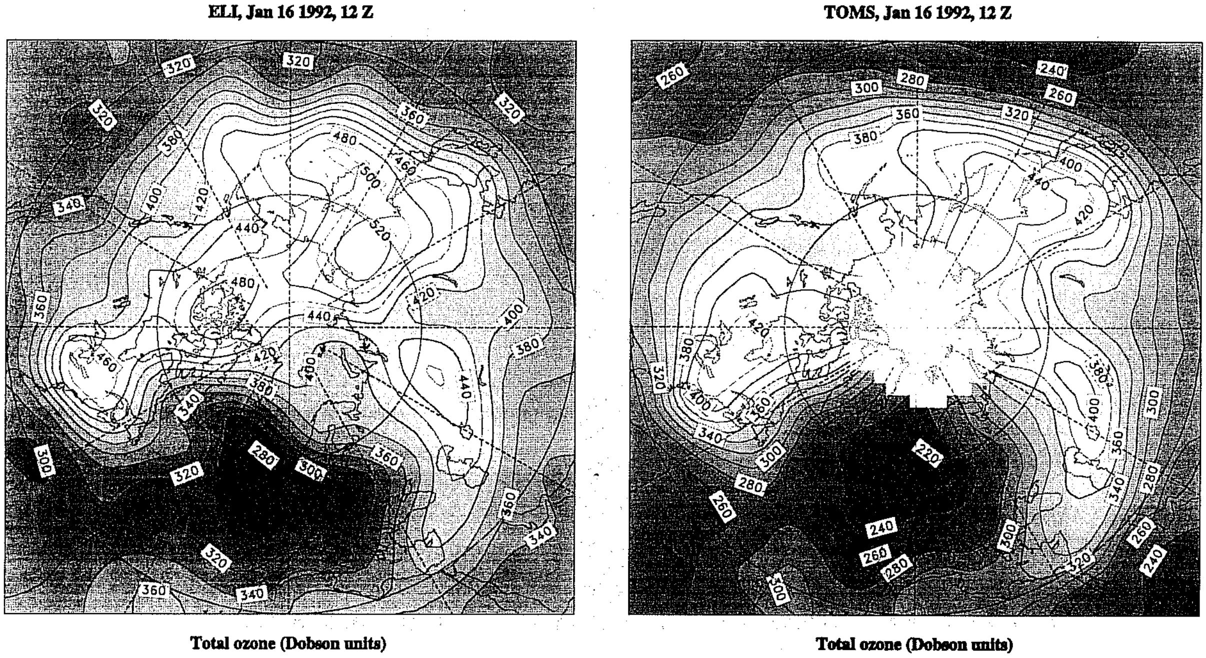


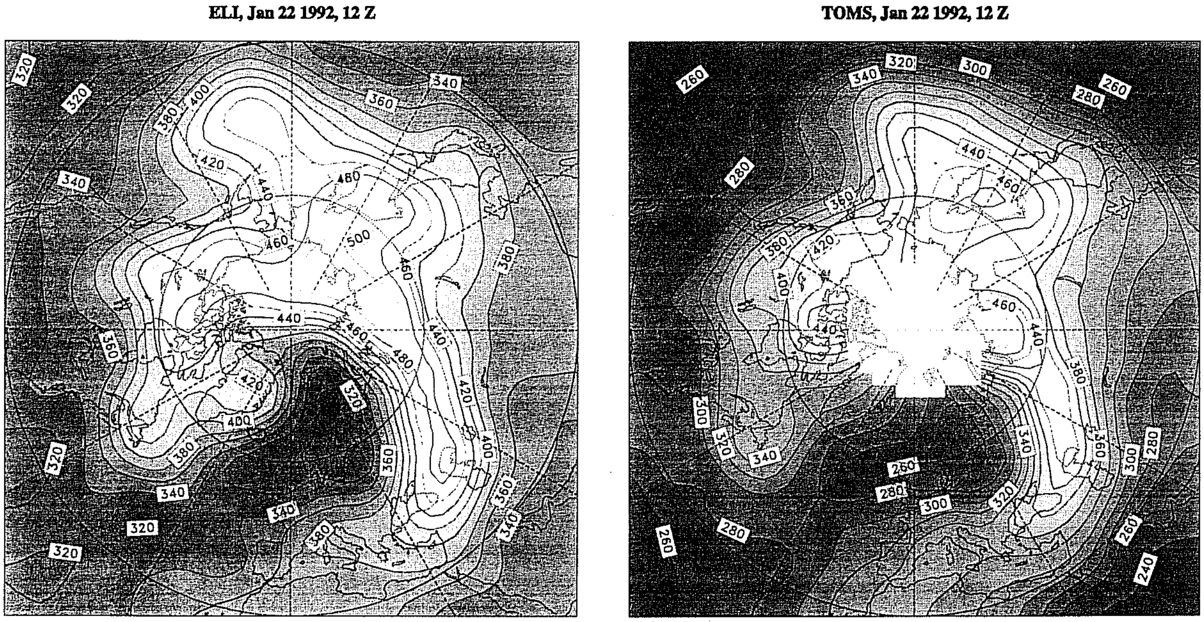
Figure 2 Total ozone on January 16, 1992, 12 Z, as (a) captured by the EPVL initialisation, and (b) as seen by the TOMS instrument

over Western Siberia by a trough of low ozone values around 90 E. Two major differences can however be pointed out between the TOMS total ozone and the synthetized L93 total ozone: One is the shape of the pattern near the polar night hole in the TOMS data, and the other is the difference in the absolute values between the two plots.

The difference near the polar night hole is probably in part an artefact of the plotting package because of the void in the data, but it may also be influenced by the well-known errors in the TOMS measurements at high solar zenith angles (Lefèvre and Cariolle, 1991). The difference in absolute values is systematic, with L93 almost always overestimating the total ozone with respect to the TOMS data. The relative overestimation is larger at lower latitudes where few or no soundings were available, and this could indicate that the background ozone field of January 1992 did not resemble the field of the two-dimensional photochemical model used in the L93 scheme at the low latitudes.

Corresponding plots of L93 and TOMS total ozone for January 22, 12 Z are shown in figure 3. Again we see that the L93 algorithm captures the overall features of the ozone field rather well with a general tendency of overestimating the total ozone. Even for this date the relative overestimation is larger for the lower latitudes.

In order for the model to start from an ozone distribution as close as possible to the real one, the ozone field produced by the L93 scheme was normalized so that the vertical integral would



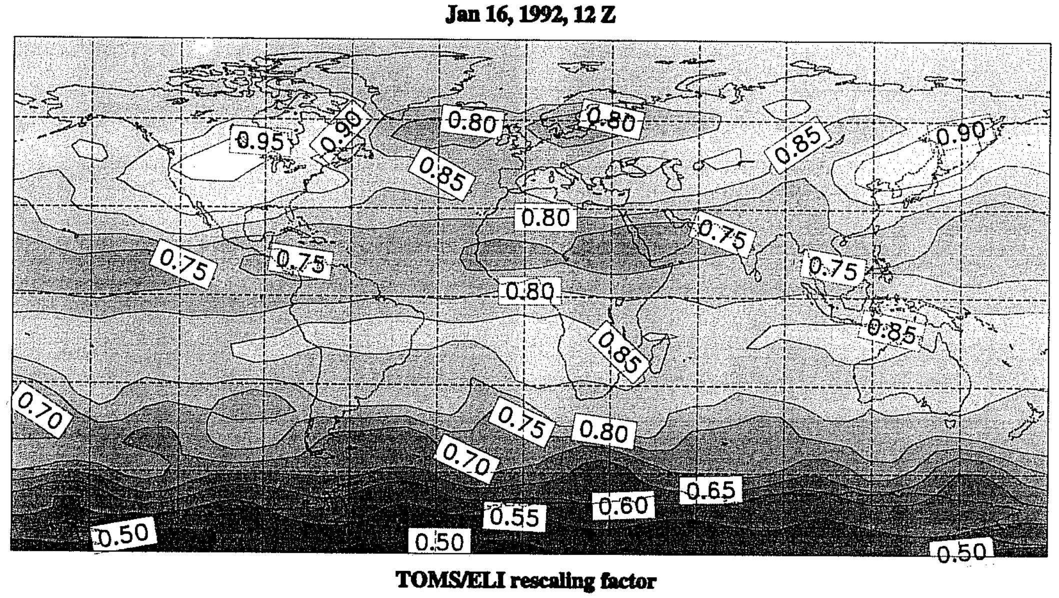
Total ozone (Dobson units)

Total ozone (Dobson units)

Figure 3 Same as fig. 2; but for January 22, 1992, 12 Z.

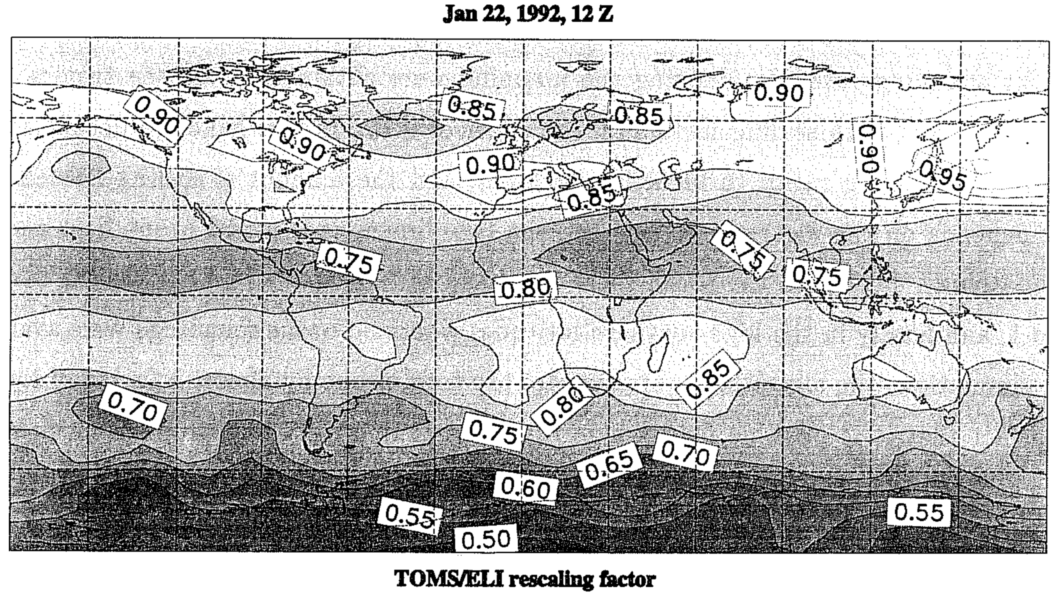
correspond to the TOMS data. This normalisation was done using a smoothing algorithm to avoid large differences in the scaling between neighbouring points caused by systematic errors in the TOMS data or by regions with missing data. The field of normalisation factors for January 16 is shown in figure 4, while that for January 22 is shown in figure 5. It is seen that the rescaling needed is closest to 1 in the northern high latitudes, that is in the region where the soundings used for defining the mapping were obtained. Over the tropics there is a latitude band with scaling factors on the order of 0.75. In this band we do not expect PV and ozone mixing ratios to be well correlated, and the amount of scaling needed thus mainly depends on the discrepancy between the two-dimensional model ozone field and the real climatology. Futher to the south there is a band of latitudes where the scaling is again close to 1, and finally in the high southern latitudes where no ozone soundings were available for our simulations the algorithm overestimates the total ozone by almost a factor of two.

The fact that it is possible for an algorithm like that of L93 to reproduce most of the prominent features in the total ozone field agrees well with the results of Allaart et al. (1993). However, in the light of their results, it may seem somewhat surprising that the algorithm should produce so consistent an overestimation of the total ozone. A simple test has shown that the major part of this discrepancy can be made to disappear simply by scaling the ozone mixing ratio of the top levels (ie. all levels above the top analysis level at 10 hPa) with a factor of 0.7. Such a rescaling does not have a very sound physical basis, but the success of it


Jan 16, 1992, 12 Z

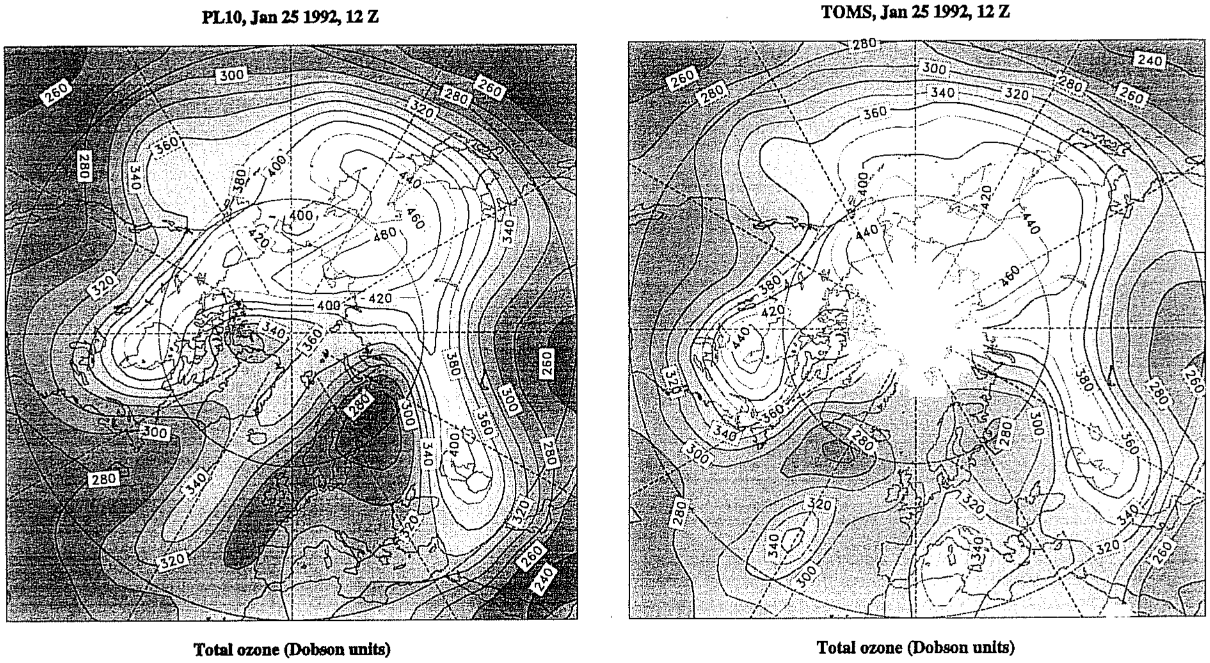
TOMS/ELI rescaling factor

Figure 4 ELI/TOMS total ozone ratio on January 16; used for rescaling the ELI ozone mixing ratios prior to model run.


Jan 22, 1992, 12 Z

TOMS/ELI rescaling factor

Figure 5 Same as fig. 4, but for January 22.



PL10, Jan 25 1992, 12 Z

TOMS, Jan 25 1992, 12 Z

Total ozone (Dobson units)

Total ozone (Dobson units)

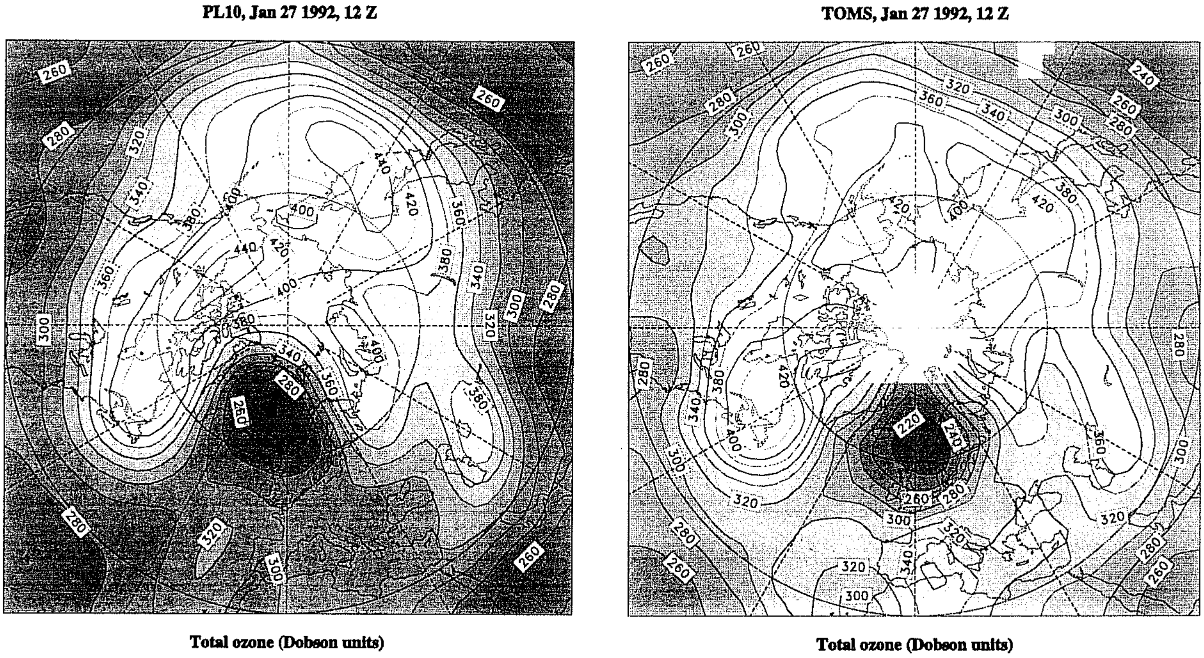
Figure 6 Total ozone on January 25, 12 Z, from (a) Arpege simulation, and (b) TOMS interpolated to corresponding Gaussian T42 grid

does indicate that the problem is likely to be caused mainly by the lack of data in the middle and upper stratosphere.

In figures 6, 7, and 8 the total ozone forecast of the model starting from the January 22, 12 Z fields is shown together with the TOMS validation data for 72 h, 120 h, and 168 h. After three days of simulation (figure 6) the model is still in good agreement with the TOMS data. The error in the field over the North Atlantic is presumably related to errors in the initial field over the subtropical regions rather than to errors in the dynamics, since we do not have reason to believe the model to go particularly wrong here.

On January 27 (figure 7) the mini-hole is fully developed and has started moving across the Scandinavian peninsula. The lowest simulated value is 235 Dobson units (DU), while the TOMS data had a minima some 20 DU lower. This difference is consistent with what Orsolini et al. (1993) found in a high resolution (T106) simulation with the same GCM as the one used here, but with their modified version of the R92 ozone initialisation.

Finally, after 7 days of simulation (figure 8) the simulated ozone field has started drifting away from the observations. Only the smallest wavenumbers can now be said to be captured by the model. This is entirely consistent with the dynamical evolution of the model run, as can be seen from figures 9 and 10 that show the 200 hPa height forecasts and the corresponding ECMWF analysis after 72 and 168 hours of simulation, respectively. The 3 day forecast (figure

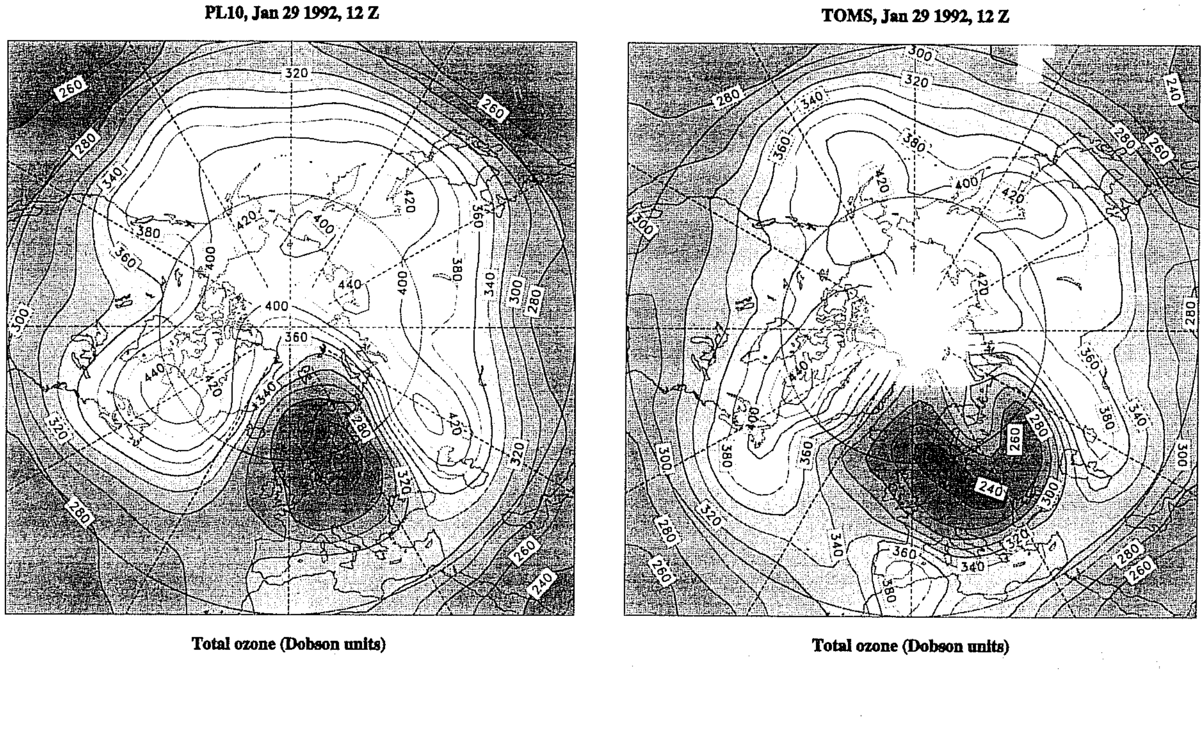

PL10, Jan 27 1992, 12 Z

TOMS, Jan 27 1992, 12 Z

Total ozone (Dobson units)

Total ozone (Dobson units)

Figure 7 Same as fig. 6, but for January 27, 12 Z

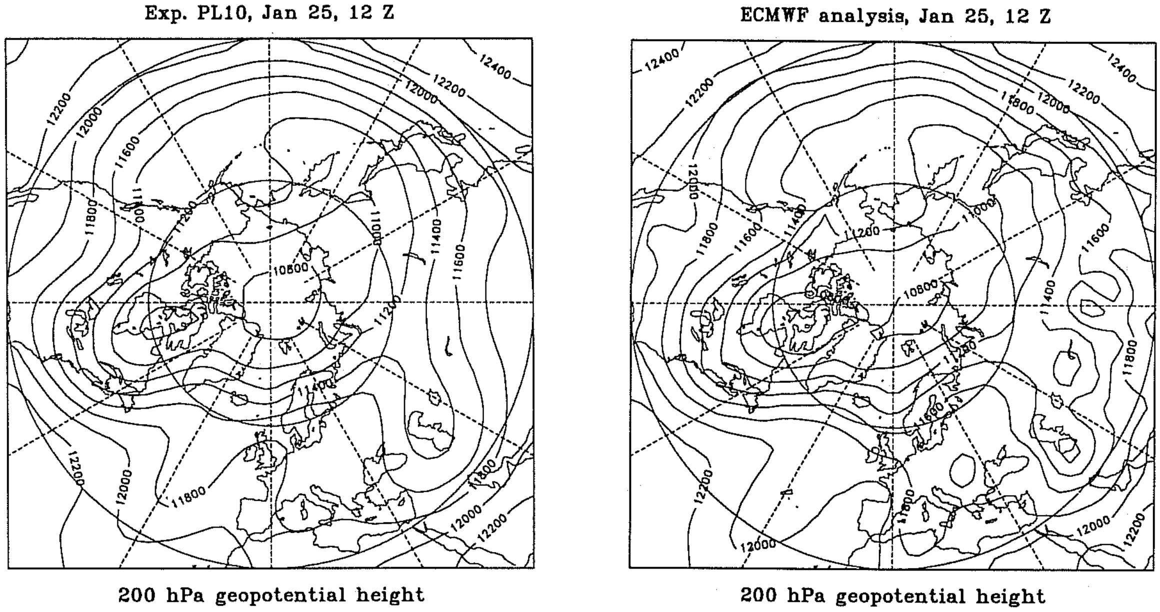

PL10, Jan 29 1992, 12 Z

TOMS, Jan 29 1992, 12 Z

Total ozone (Dobson units)

Total ozone (Dobson units)

Figure 8 Same as fig. 6, but for January 29, 12 Z.



Exp. PL10, Jan 25, 12 Z

200 hPa geopotential height

ECMWF analysis, Jan 25, 12 Z

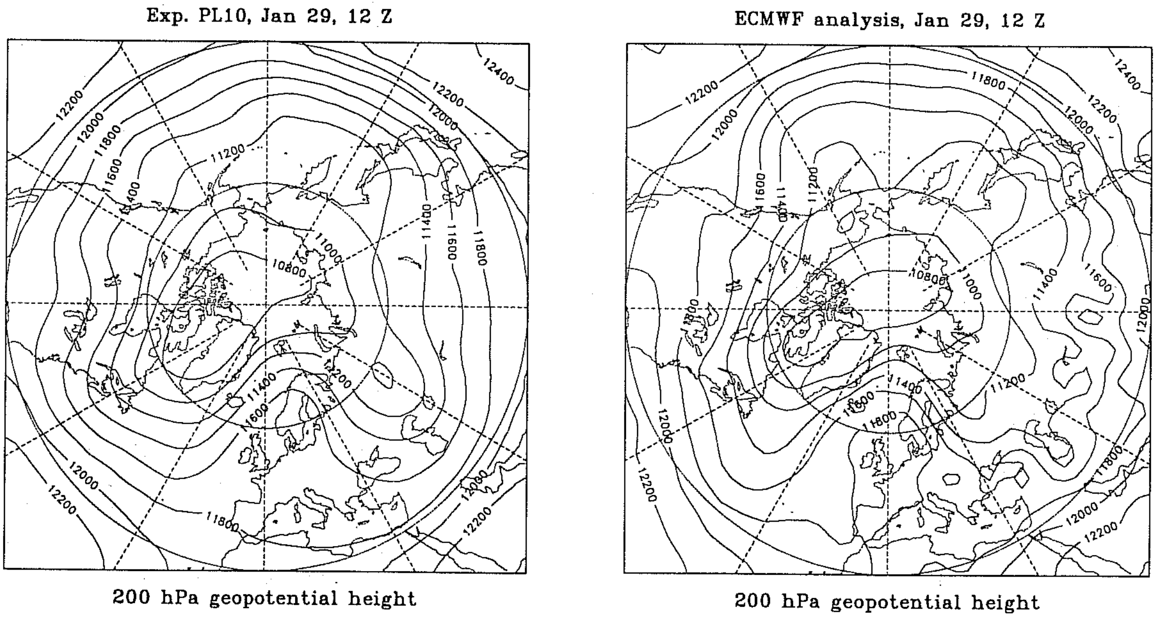
200 hPa geopotential height

Figure 9 200 hPa height field on January 25, 1992, 12 Z from Arpege simulation (a), and from ECMWF analysis (b).

9) is still in relatively good agreement with the analysis, while the 7 day forecast (figure 10) has lost a significant amount of detail in the higher wavenumbers.

In figures 11 and 12 we show the RMS difference between the total ozone forecast and the TOMS data as a function of time for the latitude band between 20 N and 65 N . We see that the RMS error after 24 hours of simulation is on the order of 15 DU, and at the end of the forecast period it is on the order of 35 to 40 DU. This can be compared to the RMS difference between the TOMS data and the ozone 'climatology', here defined to be the mean of the TOMS data for January 1992 and 1993, since these years have been rather different from the previous years. The typical RMS error of using this climatology for forecasting is on the order of 37 DU, and this limit is here passed on day 7 or 8 of the forecast.

In figures 11 and 12 the dotted lines show the RMS error of the ozone forecast when 'raw' rather than time-interpolated TOMS data are used for initialisation as well as for the subsequent verification. This shows that even a very naive approach to dealing with the asynoptic nature of the TOMS data yields a reduction of about 5 DU in the error, here corresponding to one third of the error in the 24 hour forecast. The difference between the forecast errors for the raw versus the time interpolated TOMS data remains essentially constant throughout the range of the simulation, which leads one to expect that this order of magnitude is typical for the season.



Exp. PL10, Jan 29, 12 Z

200 hPa geopotential height

ECMWF analysis, Jan 29, 12 Z

200 hPa geopotential height

Figure 10 Same as fig. 9, but for January 29, 1992, 12 Z.

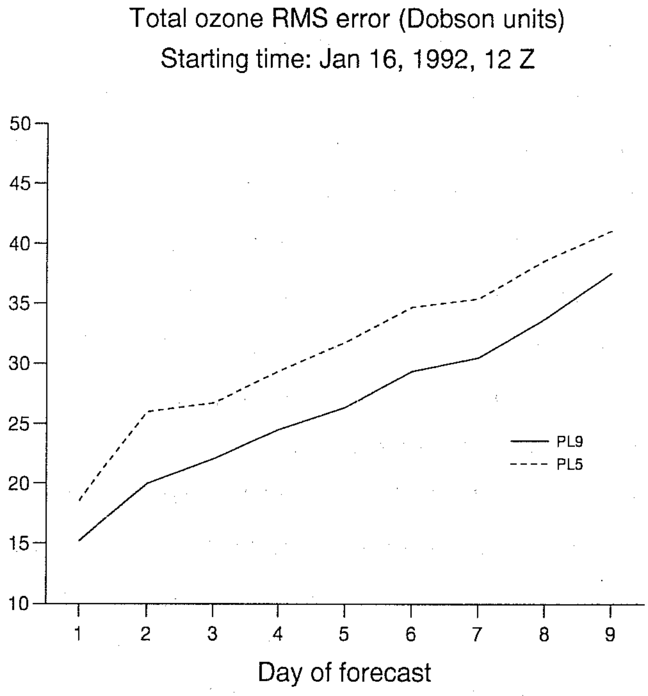


Figure 11 RMS error of total ozone forecast (defined as RMS of simulated minus TOMS total ozone) as a function of time for forecast starting on January 16. Full line shows time-interpolated TOMS data, dotted line shows raw TOMS data.

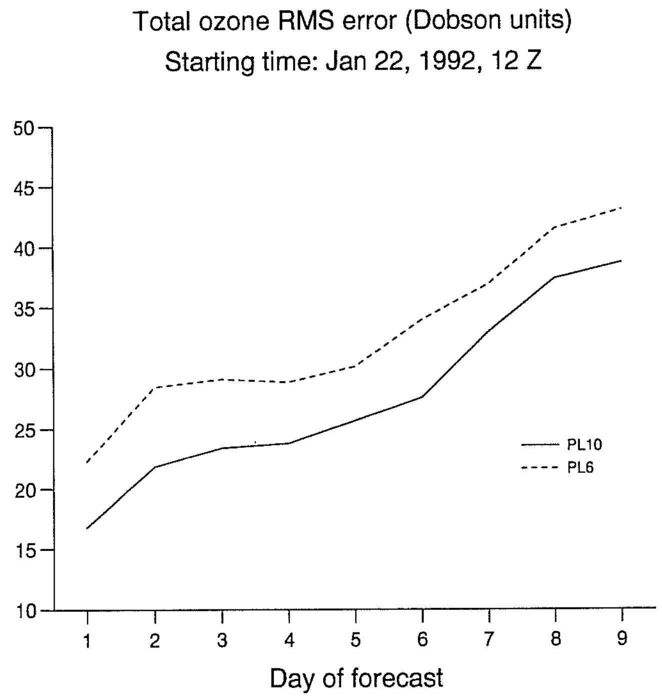


Figure 12 Same as fig. 11, but for forecast starting on January 22.

From the point of view of operational numerical weather prediction the main interest of ozone forecasting probably lies in the hope that errors in the ozone forecast might contain useful information about errors in the dynamics. This would allow us to make use of the fact that total ozone is a relatively easily observable quantity.

As an attempt to see whether or not this is likely to be true we have calculated the spatial correlation between the normalized error of the total ozone forecast on one hand (again defined relative to the TOMS data) and the normalized error in the geopotential height forecast on the other hand (defined as forecast minus ECMWF analysis) for the same latitude band as the one used in figures 9 and 10. The time evolution of the correlation coefficients are shown in figures 13 and 14 for four different pressure levels, two in the troposphere (850 hPa and 500 hPA), and two in the stratosphere (200 hPa and 50 hPa), of which the former presumably occasionally cuts through the tropopause.

We see that for all the levels shown here the errors start out as being nearly uncorrelated, and that for both forecasts the error at the extreme levels (850 hPa and 50 hPa) remains largely uncorrelated with the error in the ozone forecast. For the two intermediate levels there is a tendency towards a negative correlation coefficient of increasing magnitude. This is most clearly seen for the 200 hPa level that on average is closest to the tropopause. That the correlation is negative means that when the geopotential height field is too high the total

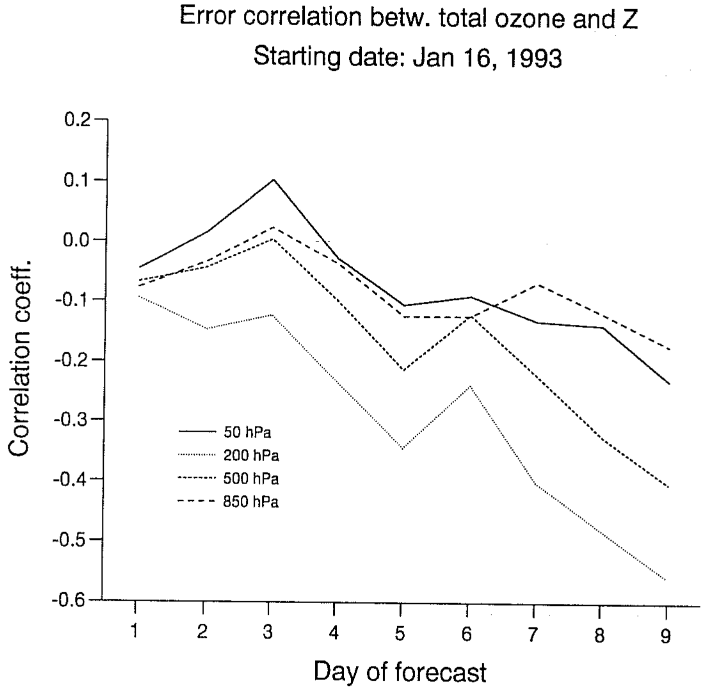


Figure 13 Correlation coefficient for total ozone forecast error and geopotental height forecast error as a function of time for forecast starting on January 16. Four different pressure levels are shown.

ozone is too low. This is in good agreement with what is already known about the relationship between ozone and dynamics (see e.g. Vaughan and Price, 1991, and references herein). The interesting thing to notice here is rather that part of the error in the ozone forecast can clearly be attributed to errors in the dynamical forecast. It is difficult from this kind of calculations to tell exactly how much of the ozone forecast error is caused by this. Presumably dynamical forecast errors at all levels from 500 hPa up to 50 hPa contribute with various weights, and while the forecast errors at the various pressure levels are certainly intercorrelated, they do not in general have a completely barotropic structure. The contributions are thus neither additive nor identical.

Figure 15 shows the correlation between the total ozone and the geopotential height fields themselves rather than the error correlation. The correlation is shown for the ECMWF analysis fields. Again we see that the two levels closest to the tropopause show the highest correlation with the total ozone, but the magnitude of the correlation remains nearly constant in time. The height field in the lower troposphere shows a moderate correlation with total ozone, consistent with what was already observed by Dobson and coworkers several decades ago (refs.) concerning the relationship between surface pressure and total ozone, while the 50

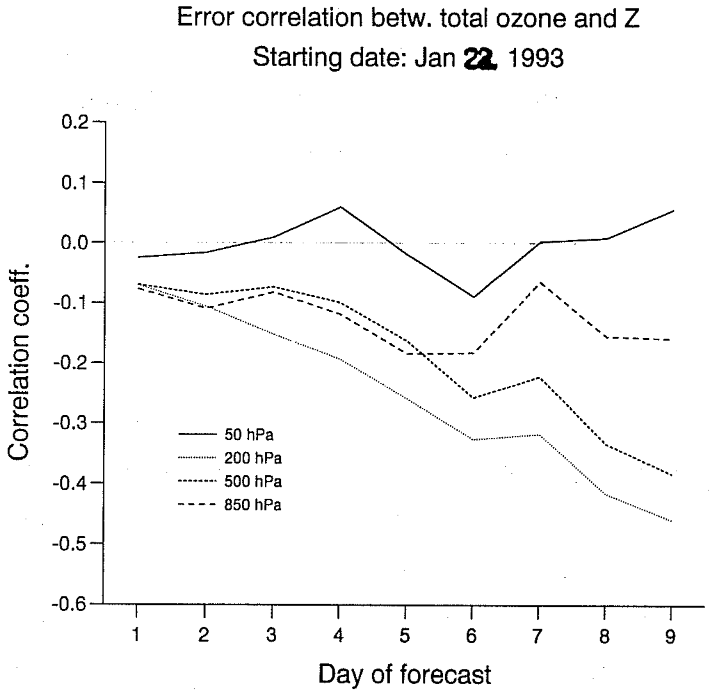


Figure 14 Same as fig. 13, but for forecast starting on January 22.

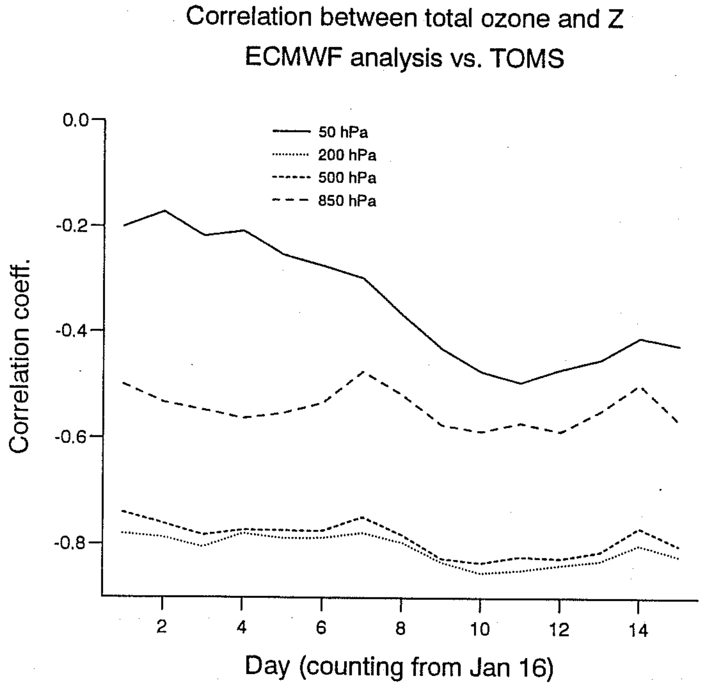


Figure 15 Correlation coefficient between analyzed geopotential heights and TOMS total ozone for the period from January 16 through January 31, 1992, for the same four pressure levels as Cin figs. 13 and 14.

hPa level in the middle stratosphere has a rather low correlation. This figure thus in a sense confirms the fact that total ozone is mainly governed by tropopause level dynamics, but it also indicates that the time evolutions seen in the figures 13 and 14 are real. No slow drift in the correlations can be seen from figure 15 at the 200 hPa and 500 hPa levels.

SUMMARY AND CONCLUSIONS

We have shown two 10 day simulations of the general atmospheric circulation in January 1992. The simulations were done with a model configuration biased towards giving a good simulation of the stratospheric circulation, that is with most of the vertical levels in the stratosphere, and the model furthermore includes ozone as a forecast variable.

The simulations were done partly in order to improve our knowledge of the dynamical processes relevant for the ozone issue, and partly in order to test a new method of calculating the three-dimensional ozone distribution at the initial model time. The ELI method (Equivalent PV Latitude Initialisation) used is based on the concept of ozone mixing ratios being well correlated with the potential vorticity on isentropic surfaces in the extratropical atmosphere between the 500 and 50 hPa levels.In our application of the method we have used ECMWF analysis fields, EASOE ozone soundings, and TOMS total ozone to calculate the initial ozone distributions.

In validating the results we have put special emphasis on the total ozone forecast, and it is shown that there is skill in the total ozone forecast up to 7 to 8 days ahead. Assuming that the model equation for ozone mixing ratios is perfect, and that the observation error of the TOMS data is zero, two factors contribute to the subsequent ozone forecast error: (i) Imperfect knowledge of the initial ozone distribution, and (ii) The dynamical forecast error.

Even though the dynamics play an important part in the ELI method through the use of the ECMWF analysis fields, the method as implemented here still has some weaknesses that are independent of the dynamical forecast error: There is a lack of ozone data for the low latitudes and a lack of both ozone and analysis data for the high altitudes, and the method of dealing with the asynoptic TOMS data is at best rudimentary. However, it is now clear that a substantial part of the ozone forecast error is directly caused by errors in the dynamical forecast, and not by the ozone initialisation. This is shown by the fact that the forecast error for ozone exhibits a negative correlation with the forecast error for geopotential height near the tropopause, the magnitude of which increases with time. It is further supported by the fact that the useful forecast range for ozone is of the same length as that for the dynamics.

The simulations described here have been based on TOMS data. Total ozone can be derived also from TOVS data, albeit with lower a precision. Contrary to TOMS data, data from the TOVS instruments are available within a delay that allows using them for operational purposes, and as furthermore no global-coverage TOMS instrument is presently (November 1993) operational, it seems desirable that this kind of simulations should also be done using TOVS data, to see if similar conclusions can be drawn from them.

After further refinement and validation of the ELI or a similar method of analyzing the three-dimensional ozone field, it would seem worthwhile to try to include ozone as a forecast variable in an experimtal version of an assimilation/forecast system in order to investigate the possibilities of using the ozone data for correcting the errors in the dynamical fields. The 4-dimensional variational data assimilation appears to be a well-suited framework for testing these ideas, both because of its natural capability of dealing with the asynoptic data from the polar orbiting satellites, and because of the possibility of dealing with observations of quantities that are nonlinear functions of the model variables, such as total ozone.

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