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Assimilation of MLS ozone measurements in the global three-dimensional chemistry transport model ROSE

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Abstract. A method for assimilating observations of ozone was implemented in the three-dimensional global stratospheric chemistry transport model ROSE. The model contains an extensive photochemical scheme which includes heterogeneous chemistry and uses temperature and wind fields from the UKMO (United Kingdom Meteorological Office) stratospheric analysis.

Ozone measurements obtained by the Microwave Limb Sounder (MLS) on board the Upper Atmosphere Research Satellite (UARS) were assimilated in the model using the sequential statistical interpolation approach. The analysis is performed using a time invariant background error covariance matrix that only includes horizontal covariances. Results from a sixty day simulation are presented and it is shown that assimilation of the MLS observations results in improved global three-dimensional distributions of ozone as seen from comparisons with MLS data not assimilated in the model. For further validation, the stratospheric total ozone fields computed from the analysis are compared with the TOVS total ozone measurements and it is shown that they agree within the uncertainty of the data.

Introduction

The Upper Atmosphere Research Satellite launched in September of 1991 has supplied a vast amount of unique measurements which can potentially extend our knowledge of atmospheric chemistry and dynamics and help to improve our abilities to numerically simulate various atmospheric processes. However, the nature of global satellite observations often makes comparisons of satellite data with model results and incorporation of observations into models cumbersome and difficult. While it is possible to "map" satellite data onto regular time-space grids using various empirical mathematical interpolation techniques, it is highly desirable to have a more rigorous methodology. The need for such framework will likely become more and more obvious in the future as new space-borne instruments are deployed.

In this paper we apply mathematical techniques of the estimation and inverse problem theory, often referred to as data assimilation, for mapping of global satellite observations and incorporating such observations into numerical models. The main objective is to demonstrate applicability of these methods to atmospheric photochemical modeling and study impact of the assimilation on model results.

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Model and data description

The off-line version of the three-dimensional chemistry transport model ROSE ("Research for Ozone in the Stratosphere and its Evolution"; Rose and Brasseur, 1989), is used in this work for assimilation of global satellite ozone measurements. The off-line version of ROSE is driven by the daily UKMO stratospheric analysis data calculated for the UARS mission [Swinbank and O'Neill, 1994]. The horizontal resolution of the model is 5^o latitude and 11.25^o longitude. It has 19 layers in the vertical from 316 mb up to 0.316 mb. These pressure levels coincide with the UARS/MLS and the UKMO stratospheric analysis levels. The transport scheme is semi-Lagrangian, described in Smolarkiewicz and Rasch (1991). The (photo)chemical scheme includes oxygen, nitrogen, carbon, chlorine, hydrogen, and bromine species. The model contains an extensive set of photochemical reactions and includes heterogeneous processes.

The MLS instrument on board UARS (Reber et al., 1993) observes the microwave atmospheric limb emissions on a global scale during both day and night. The instrument measures profiles of several trace gases including O_3 with vertical resolution of about 6 km. The retrievals are made on alternate standard UARS pressure levels. The retrieved mixing ratios are then interpolated to the standard UARS pressure levels which coincide with the model vertical levels.

It is believed that the MLS version 4 ozone data used in this study are reliable from about 46 to 0.46 hPa (Froidevaux et al., 1996). In most cases the accuracy and approximate precision are 0.3-0.4 ppmv and 0.2-0.3 ppmv respectively as estimated from the UARS/MLS Data Quality Document (http://mls.jpl.nasa.gov/lucien/daac_document_v4).

The TIROS Operational Vertical Sounder (TOVS) total ozone measurements used for comparisons with the assimilation experiments are from the National Oceanic and Atmospheric Administration (NOAA) satellites NOAA 11 and 12 (Smith et al., 1979). The TOVS total ozone data shown here are mapped as described in Levelt et al. (1996). The errors of the mapping procedure have been shown to be negligible (M. Allaart, personal communication).

Data assimilation

The mathematical apparatus used in this work can be found, for instance, in Lorenc (1986). Let vector x_b, often called the background, represent concentrations of ozone at the model grid points. The uncertainties and the error correlation for the simulated tracer field x_b are given by the background error covariance matrix, B. Its diagonal elements are the variances of the elements of x_b and the off-diagonal elements are the error covariances of different elements of x_b. In a similar fashion, the available observations within one analysis interval can be arranged in a vector y with the error covariance given by matrix O. A linear interpolation is

used to define a transformation from the model grid to the observations, by means of observational operator H, which allows one to estimate the model predicted ozone values at the observation locations: Hx_b. The best estimate of the state, ozone concentrations in our case, is obtained from the background x_b and the available observations y as (Lorenc, 1986):

$$x_a = x_b + K(y - Hx_b)$$

where matrix K, often referred to as the Kalman gain matrix, is given by

$$K = BH^T(HBH^T + O)^{-1}$$

The analysis described by the above equations is performed every day using observations collected for up to 12 hours before and after the analysis time. Once the analysis is completed, values of elements of x_a are used as initial conditions for the model for the next 24 hour integration. Concentrations of other chemical species in the model are allowed to adjust to the ozone concentration according to the model's (photo)chemical equations. The model vertical levels coincide with the standard UARS pressure levels and the analysis is performed independently at each level.

The observational error covariance matrix O is assumed to be diagonal and the values of the diagonal elements (variances) are computed from the reported uncertainties of the MLS data as follows:

$$O_{ii} = {\sigma_{ii}}^2 + (0.3ppmv)^2$$

Here σ_{ii} is an approximate lower bound of the total uncertainty at each level as given by the MLS data quality indicator and the value of 0.3 ppmv is the average 1-σ uncertainty calculated from statistical comparisons of the MLS measurements with independent correlative data. Description of both these quantities are obtained from the MLS Data Quality Document. In most cases, the observational error variance amounts to about 5-10% of the measured ozone mixing ratio.

It is assumed that the background error covariances do not change with time. All diagonal elements of B are set to 10% of the forecasted ozone mixing ratio. The absolute values of the observational and background variances imply that in the 31 to 1 mb region the relative weights of the observations are 1-4 times the weights of the background. Below 31 mb and above 1 mb errors of the MLS data increase and the relative weights of the observations decrease accordingly, depending on the quality of a particular observation. The functional dependence of the background error covariances B on the horizontal separation between two locations is described by the Gaussian function with a fixed correlation length of 1000 km.

Realistic estimates of the background error covariance B present a difficult problem. Although calculations of forward evolution of the forecast error in numerical transport models are possible in some cases (Lyster et al., 1997), such calculations are extremely computationally expensive. By setting the background error variances to the upper limit of the observational variance (10%) and by keeping the background error covariances constant in time we effectively replace the simulated ozone with MLS measurements after a few analysis cycles in the regions where observations are available. Therefore, quality of the MLS data is the most important factor determining quality of our results.

Performing the analysis at each level independently implies that the background and observational error covariances in the vertical direction are set to zero. This is not a valid assumption as there exists vertical transport in the model and MLS observations at different levels are not completely independent. Due to the high density of the MLS data correct determination of the vertical and horizontal error covariances is probably not very crucial. Ultimately, however, the errors of the analysis due to these imposed simplifications and other factors can be estimated by performing systematic comparisons with independent data.

Results and discussion

The model integration started 4th of January 1996 with zonally averaged tracer fields as the initial conditions. Figure 1 shows results at 10 mb for January 4th, January 18th, and February 1st. The first column shows ozone distribution obtained in the control model run without incorporation of the MLS data. The second column presents results of assimilation of the MLS data up to but not including the day on which the results are displayed. The third column shows MLS ozone observations for that day. Note, that the displayed MLS measurements were not yet used and are thus independent of the assimilation results shown in the second column.

Both the control model run and the assimilation analysis significantly modify the initial ozone distribution and make it more realistic. The general features of the ozone distribution are approximately the same in both cases. However, absolute values of the ozone mixing ratios often differ significantly, with the assimilation analysis being closer to the observations. This is not very surprising since both simulations use the same realistic UKMO dynamical information and therefore, for instance, they are able to reproduce the intrusions of the ozone rich low latitude air into the North polar regions seen on both January 18th and February 1st. Absolute values of ozone are determined mostly by vertical transport and photochemical processes and inclusion of MLS data clearly helps to correct to some extend model deficiencies associated with the treatment of these processes.

A number of simplifications have been introduced in the analysis in section 3. While it is difficult to predict the impact of each of these simplifications, it is possible to assess the quality of our final results by computing RMS deviations between the analysis and the MLS observations not yet used in the assimilation. In order to estimate the average errors of our results we have computed RMS differences between the assimilation analysis (second column of figure 1) and observations not yet used in the assimilation (third column of figure 1) for each latitude band. Same calculations were performed for the control model run, performed without incorporation of the MLS data. The results are shown in figure 2. Blank areas in this figure indicate times/latitudes where no MLS measurements are available. Clearly, the RMS values are lower in the case of the assimilation analysis where zonal mean deviations from observations generally do not exceed 5-10% in between 30^{o}N and 30^{o}S. These deviations increase at high latitudes, poleward of about 50^o in both hemispheres. Obviously, in these regions the model is unable to adequately simulate ozone. Even in these areas, however, the assimilation results are closer to the observed values with RMS deviations of about 10% as opposed to 15-

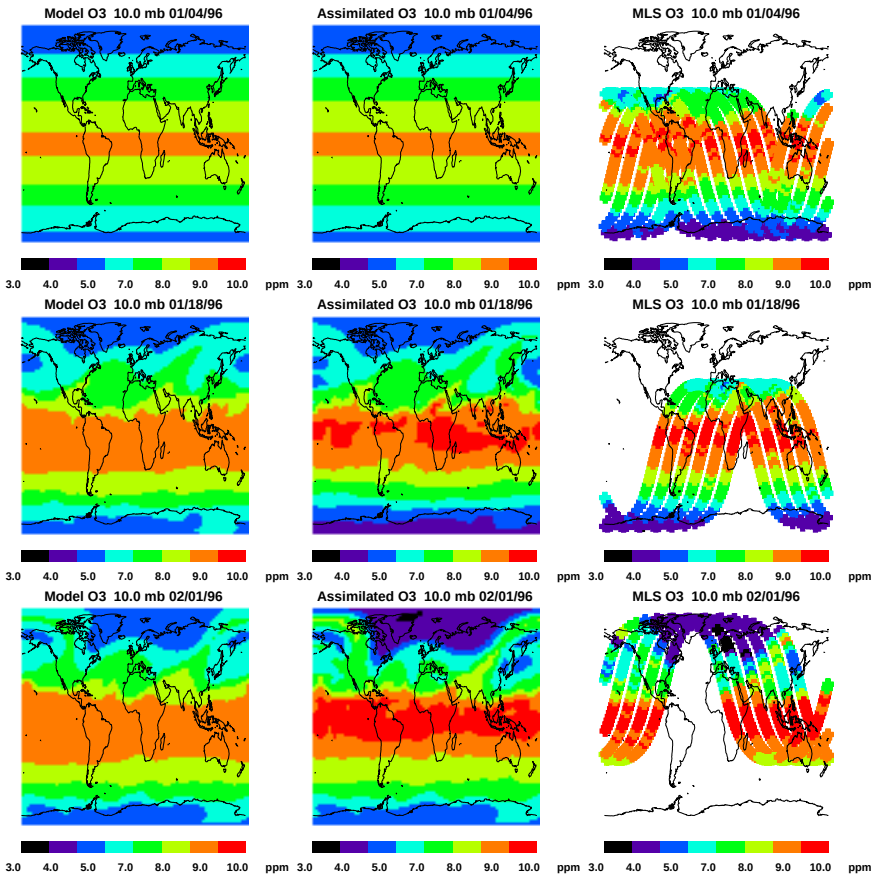

Figure 1. First column: control model run (no assimilation) for Jan 4, Jan 18, and Feb 1 of 1996; second column: results of assimilation of ozone up to but not including data for the same days; third column: MLS observations for the same days.

30% in the case of the control run. The RMS deviations for the assimilation results remain within 10%-15% in the region between 31 and 1 mb. Below 31 mb and above 1 mb the relative weights of the MLS measurements decrease as mentioned in the previous section and the RMS deviation grow accordingly, to about 70% at the 100 mb level.

Figure 3 shows differences between the stratospheric total ozone amounts computed from the model (top) and the as-

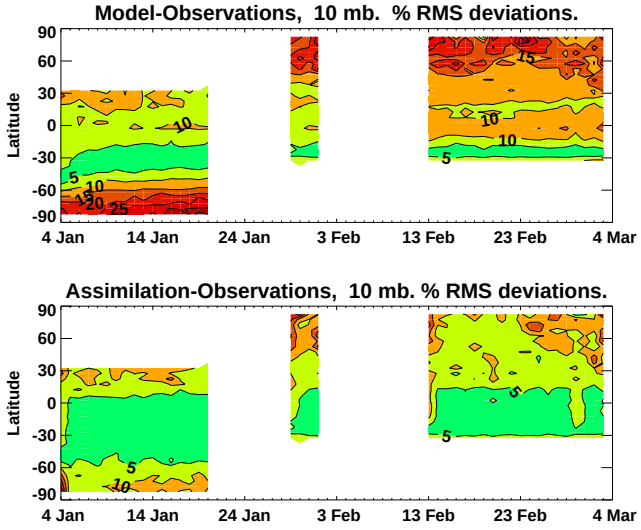

Figure 2. Zonally averaged RMS deviations from MLS measurements in % for the control model run (top) and assimilation run (bottom).

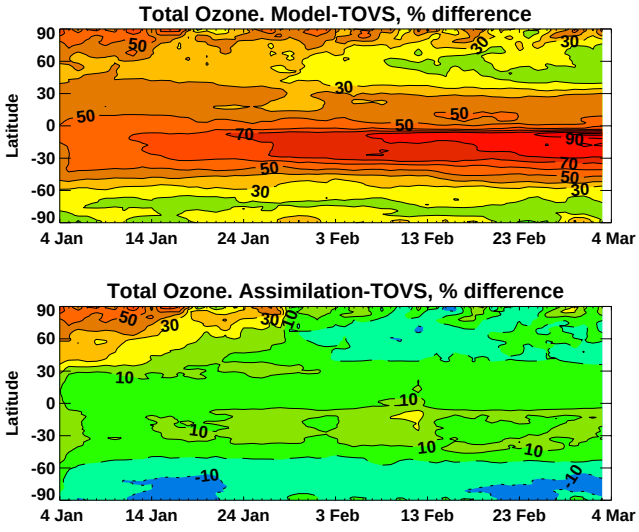

Figure 3. Difference in % between the stratospheric total ozone amount computed from the model (top) and assimilation results (bottom) and the TOVS total ozone measurements.

similated (bottom) three-dimensional fields and the TOVS total ozone data as a function of time and latitude. Clearly, results of the assimilation are in a much better agreement with TOVS than results of the control model run. Note the gradual decrease of the discrepancies between the assimilation results and TOVS data at high Northern latitudes. The differences decrease from about 50% at the beginning of the integration to about 30% by January 24. Similar behavior is seen in the top panel. As figure 2 indicates, there are no MLS measurements in the Northern Hemisphere during this time. Therefore, it appears that the observed decrease is due to the change of the initial zonally symmetric ozone distribution in the model by the UKMO winds and model chemistry. The remaining 30% discrepancy abruptly decreases to 5-10% when MLS data become available in the Northern Hemisphere (see figure 2). In the tropical and southern latitudes, where MLS measurements are available from the beginning of the integration, the differences remain near 5-10%. Note, that the computed analyzed total ozone values do not include the tropospheric amount and therefore the TOVS measurements should be slightly larger than the derived stratospheric total ozone column. This is consistent with the negative values in figure 3 in some areas at high latitudes. Some estimates show that errors of the TOVS data are about +/-15% for tropical regions and increase to about +/-50% for polar regions (http://www-eosdis.ornl.gov/FIFE/Datasets/Atmosphere/TOVS_atmos_prof.html). Given these estimates we conclude that our results appear to agree with the independent TOVS total ozone data within the measurement uncertainty. A possible explanation of the remaining differences between our results and the TOVS total ozone data is that the MLS ozone measurements are not very reliable below 46 mb (Froidevaux et al., 1996), while ozone in this region constitutes a large portion of the total column amount.

In conclusion we note that although the employed data assimilation scheme is fairly crude it clearly improves model simulations of ozone as seen from comparisons with the MLS and TOVS data. The performed research appears to be one of the first applications of the data assimilation methodology to global, three-dimensional photochemical modeling of the atmosphere and the preliminary results are encouraging. An additional benefit of assimilating ozone observations into photochemical models is that the improved ozone distributions affect simulated distributions of other model species that photochemically depend on ozone.

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