

Data assimilation of stratospheric ozone using a high-resolution transport model

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[1] We describe a method for assimilating sequentially tracer measurements in isentropic chemistry-transport models (CTMs) of the stratosphere. The parametrisation of the forecast error covariance and its evolution is largely based on simplifications described in *Menard and Chang* [2000] and *Khattatov et al.* [2000]. The model used here is a high resolution isentropic advection model which is driven by ECMWF (European Center for Medium range Weather Forecast) meteorological analyses. The assimilation on isentropic surfaces allow us to exploit the well-established correlation between tracer mixing ratio and potential vorticity in the formulation of the forecast error covariance. Multiple 20-day sequential assimilations of MLS (Microwave Limb Sounder onboard UARS satellite) ozone data during an ozone depletion event are performed. χ^2 (chi-square) and OmF (observation minus forecast) statistics are used to optimise the assimilation system by adjusting parameters of the error covariance. The quality of the analysis is found to be significantly improved when the strong correlation between ozone and potential vorticity is taken into account. *INDEX TERMS*: 1635 Global Change: Oceans (4203); 4203 Oceanography: General: Analytical modeling; 4267 Oceanography: General: Paleoceanography; 4806 Oceanography: Biological and Chemical: Carbon cycling; 4870 Oceanography: Biological and Chemical: Stable isotopes

1. Introduction

[2] The role of transport processes in regulating the chemical composition of the lower stratosphere has been studied intensively. One of the reasons is the possible role of dynamical trends in the long-term decline in total ozone observed at middle latitudes in the Northern Hemisphere [*Scientific Assessment of Ozone Depletion*, 1999]. Chemical-transport models (CTMs) are key analysis tools in transport studies. Their evolving 3-D fields can aid considerably in investigating the transport of tracers in the atmosphere. However, CTMs have deficiencies which are not necessarily well characterised. Therefore it is important to develop rigorous approaches to assess, constrain and possibly combine them with observational data. Data assimilation attempts to combine the information contained in CTMs and observations in an optimal way in order to produce a comprehensive and consistent picture of the atmosphere. It is increasingly used in the scientific exploitation of satellite chemical observations. Our attention is focused here on the Kalman filter which has been applied successfully to the assimilation of satellite tracer observations [*Levelt et al.*, 1998, *Menard et al.*,

2000, *Khattatov et al.*, 2000]. The purpose of this work is to explore whether the well-established correlation between tracer mixing ratio and potential vorticity on isentropic levels [see for example *Hoskins et al.*, 1985] can be exploited in assimilation and, in particular, be used to specify some flow-dependency in the forecast error covariance. It has already been shown that high resolution transport models are able to reproduce fairly accurately many small-scale features observed in chemical tracer distributions using potential vorticity as a proxy [*Orsolini et al.*, 1997; *Hauchecorne et al.*, 2001]. The same authors pointed out that such models can represent observed filamentary structures down to scales much smaller than the scales resolved in the advecting wind fields. For instance, in the case of tropospheric baroclinic eddies, *Methven and Hoskins* [1999] showed that the ratio between the smaller scale resolved in the wind field and the size of the smallest scales reproduced in the tracer field is at least 6. The sequential assimilation algorithm used in this work, originally developed by *Hauchecorne et al.* [1998] and modified according to *Khattatov et al.* [2000] study, is designed to assimilate measurements of long-lived stratospheric chemical species such as ozone in the lower stratosphere. It is able to estimate the errors of the analysis and predict their evolution. The interest of data assimilation on isentropic levels using an advection model is twofold. First of all, this allows the additional information originating from the correlation between tracer and potential vorticity to be exploited in the assimilation algorithm. Second, the relatively low computational cost of the model makes it possible to run it at high resolutions and describe in details the distribution of long-lived chemical species. This cannot be achieved with a full 3-D CTM. The high resolution could open the way to a more effective assimilation of satellite slant columns data which have an effective horizontal resolution higher than the current assimilating CTMs. The present paper illustrates the applicability of this approach. The second section describes the model and the formulation of the assimilation algorithm. The determination of the assimilation parameters is explained in the third section. The results are presented and discussed in the following section. Some of the limitations and the possible improvements of our approach are highlighted in the conclusion.

2. Assimilation

2.1. MIMOSA Advection Model

[3] The MIMOSA model (Modèle Isentropique de transport Mésoéchelle de l'Ozone Stratosphérique par Advection) is an advection model on isentropic surfaces. The horizontal resolution is 0.5° latitude \times 0.5° longitude. The model domain is centred onto the North Pole and covers the Northern Hemisphere down to 30° N. The advection scheme is semi-lagrangian with a timestep of 1 hour. The regridding onto the original orthonormal grid is performed every 3 hours. The model is driven by ECMWF (European Center for Medium Range Weather Forecast) meteorological analyses at a resolution of $2.5^\circ \times 2.5^\circ$. A part from the ozone tracer, potential

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vorticity (PV) is also advected. The diabatic evolution of PV is taken into account by relaxing the model PV towards the PV calculated from the ECMWF fields with a relaxation time of 10 days. The accuracy of the model has been evaluated by *Hauchecorne et al.* [2001] and validated against airborne lidar measurements within the framework of the METRO (MERidional TRansport of Ozone in the lower stratosphere) EU project [*Heese et al.*, 2001].

2.2. Assimilation Algorithm

[4] A complete description of Kalman filtering and sequential assimilation is beyond the scope of the present paper but can be found in *Daley* [1991] or *Menard et al.* [2000]. Here we only provide a brief outline of this approach. The best estimate of the state of the atmosphere, for instance an atmospheric tracer concentration field, is derived from a linear weighted interpolation of the background state vector \mathbf{x}_b and vector of observations \mathbf{y} according to

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}(\mathbf{y} - \mathbf{H}(\mathbf{x}_b)) \quad (1)$$

$$\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{O} + \mathbf{R})^{-1} \quad (2)$$

where \mathbf{x}_a is the analysis, \mathbf{H} is the observation operator, \mathbf{K} is the so-called Kalman gain, or weight, matrix, \mathbf{B} is the covariance matrix of the background errors (also called forecast errors when the background is a model prediction), \mathbf{O} is the covariance matrix of the observation errors and \mathbf{R} is the covariance matrix of the representativeness errors associated with interpolation and discretisation.

[5] If \mathbf{K} is the optimal least-squares gain matrix, the covariance matrix of the analysis error \mathbf{A} simply becomes

$$\mathbf{A} = \mathbf{B} - \mathbf{K}\mathbf{B}\mathbf{H} \quad (3)$$

[6] The computational cost of the extended Kalman filter method is rather prohibitive in our case because of the large dimension of the state vector \mathbf{x} ($N_x = 86,400$ grid points). Therefore, some simplifications are required in order to reduce the dimension of \mathbf{B} [*Khattatov et al.*, 2000]. The observation errors are considered spatially and temporally uncorrelated [see *Banfield et al.*, 1995] allowing to handle each measurement separately. The time evolution of only the diagonal elements b_{ii} (variances) of the forecast error covariance matrix are computed explicitly. Off-diagonal elements b_{ij} are simply derived from diagonal elements using a correlation function f : f is assumed to be a convolution of Gaussian functions of the distance between model grid point and the measurement [*Hauchecorne et al.*, 1998]. In this work, we aim at taking into account in a simple way the state of the atmospheric flow in the formulation of the forecast error correlations. The positive impact of a flow-dependent background error correlation on an ozone analysis systems has already been pointed out [*Riishojgaard*, 1998]. In the stratosphere, air masses tend to move along contours of constant potential vorticity (PV) on isentropic surfaces. As a result, tracer mixing ratio and PV are strongly correlated on isentropic surfaces. Specifying the correlation function partly in terms of the PV field should introduce a flow-dependency in the forecast error covariance matrix and probably improve the analysis. We assume here that the correlation function can be expressed as follows:

$$f_{ij} = \exp\left(-\left(\frac{d_{ij}}{d_0} + \frac{\Delta PV_{ij}}{\Delta PV_0}\right)\right) \quad (4)$$

where d_{ij} is the distance between the grid points i and j and ΔPV_{ij} is the difference in PV between the grid points; d_0 and ΔPV_0 are

adjustable parameters which represent the correlation lengths in physical space and in PV space.

[7] The time evolution of the diagonal elements b_{ii} of the forecast error covariance matrix \mathbf{B} are calculated explicitly following the approach of *Menard and Chang* [2000]:

$$b_{ii}(t + \Delta t) = \mathbf{M}b_{ii}(t) + [q \cdot \mathbf{x}^i \cdot (t + \Delta t) \cdot \Delta t]^2 \quad (5)$$

where Δt is the timestep, \mathbf{M} is the model operator (in our case, advection and regriding), and the last term on the right-hand side represents additional errors associated with imperfections in the model; q is an adjustable parameter which controls the growth in time of the forecast error.

[8] The representativeness error covariance matrix \mathbf{R} is assumed to be diagonal and its terms r_{ii} are expressed as relative errors [*Menard and Chang*, 2000]:

$$r_{ii} = [r \cdot \mathbf{y}^i]^2 \quad (6)$$

where r is an adjustable parameter.

3. Observations

[9] We assimilate MLS (Microwave Limb Sounder) ozone measurements onboard UARS (Upper Atmosphere Research Satellite) from 10 February to 28 February 1996. 10 days of MLS data are available during the assimilation period. The meteorological conditions of that period are characterised by a stratospheric polar vortex centred above the North Pole with an ozone reduction of up to 30% at 25 km, leading to a strong latitudinal ozone gradient. The isentropic surface considered here is the 550 K level which corresponds approximatively to the 22–24 km altitude range. The length of the assimilation windows is 3 hours which gives about 160 MLS measurements to assimilate per window. In order to account for the movement of an air mass scanned by MLS between the time of observation and the time of assimilation (middle of the assimilation window) and achieve temporal coincidence, each ozone observation is advected forward or backward in time to the assimilation time and its new position is considered to be the location of the observation. The model is initialised on the 10 February 1996 with ozone fields provided by a climatology [*Fortuin and Kelder*, 1998].

3.1. Determination of Assimilation Parameters

[10] The values of the tunable parameters d_0 , ΔPV_0 , q and r are critical to the quality of the analysis. The adjustment is achieved by minimising the RMS (Root Mean Square) of the OmF (Observation minus Forecast or innovation) or using the χ^2 (chi-square) diagnostics introduced by *Menard and Chang* [2000]. The χ^2 diagnostics is a way of testing the consistency of the error covariance parametrisation by comparing the OmF error covariance estimated in the course of the analysis ($\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{O} + \mathbf{R}$) to the OmF error covariance calculated from the actual observations and the forecast ($\mathbf{y} - \mathbf{H}(\mathbf{x}_b)$). The criteria are that the value of the scalar quantity χ^2 divided by the number of observations used in the assimilation analysis should tend towards unity and should not exhibit a temporal trend [*Khattatov et al.*, 2000]. Multiple MLS assimilations are performed in order to study the sensitivity of OmFs RMS and χ^2 to the values of the assimilation parameters. Results indicate that the value of χ^2 is primarily dependent on the values of the forecast error growth parameter q and the representativeness error parameter r , and not on the values of the correlation lengths, d_0 and ΔPV_0 . Conversely, the RMS of the OmFs is found to be overwhelmingly sensitive to the values of the correlation lengths, d_0 and ΔPV_0 . Therefore, the χ^2 diagnostics is used to tune the parameters a and r and the minimisation of the RMS of OmFs

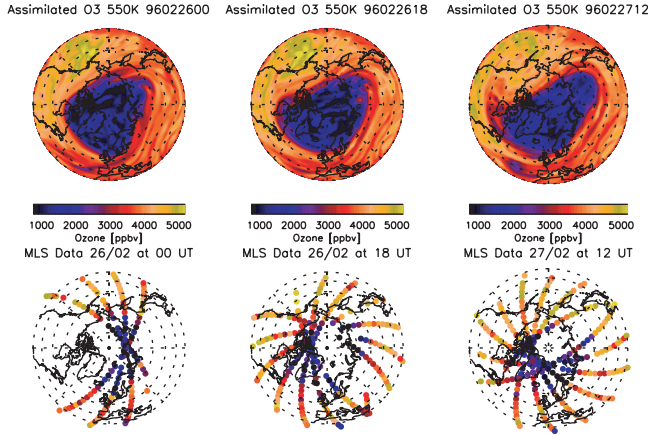


Figure 1. Ozone concentration from the MIMOSA assimilation (upper frames) and 12 hours MLS measurements (lower frames) February 26 1996, 0 UT (left frames), February 26 1996, 18 UT (center frames), and February 27 1996, 12 UT (right frames).

is used to adjust the values of the correlation lengths. *Khattatov et al.* [2000] applied a similar procedure. Satisfactory results concerning the criteria of the χ^2 test are obtained for $q = 0.0035$ per hour, $r = 0.15$ and an initial background error of 30% ($b_{ii}(t=0) = [0.3x_b(t=0)]^2$). The growth rate of the forecast error appears to be much smaller than in a previous ozone assimilation into a CTM ($q = 0.0135$ per hour) [*Khattatov et al.*, 2000]. It is not clear to us whether it is due to the much higher resolution of our model or to the fact that the advection is done on isentropic surfaces. The representativeness error ($r = 0.15$) is larger than in the *Khattatov et al.* [2000] study ($r = 0.1$). This might originate from our additional interpolation of the MLS data onto isentropic surfaces instead of assimilating directly onto the MLS pressure levels as in *Khattatov et al.* [2000]. It can also be noticed that the χ^2 does not depend significantly on the assumed value of $b_{ii}(t=0)$ after a spin up period of about 5 days. These findings are in agreement with those of *Menard et al.*'s [2000] study. The minimisation of OmFs RMS lead to $d_0 = 500$ km and $PV_0 = 1$ PV units (10^{-6} Km kg^{-1} s $^{-1}$).

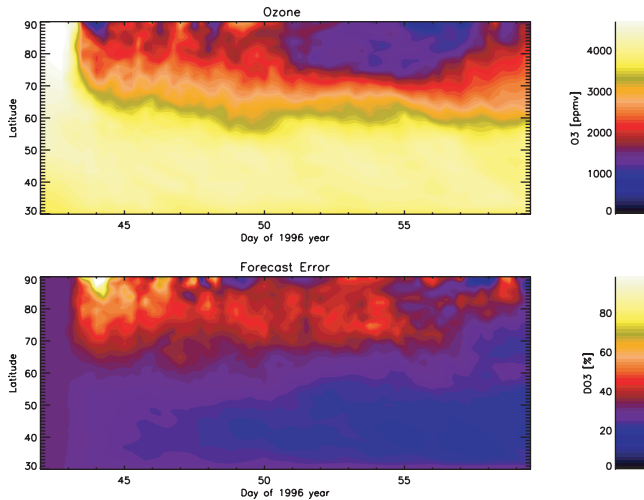


Figure 2. Time evolution of the zonal mean for the ozone concentration (upper panel), and forecast error (lower panel). MLS assimilated measurements are indicated by white bars above the x-axis.

Different formulations of the correlation function f has been tested. The best assimilation results are obtained when f depends on the distance and the PV difference as expressed in relationship (4). In addition, replacing the PV-dependency by an equivalent latitude dependency in the correlation function has no significant impact on the value of d_0 or on the value of the OmFs RMS.

4. Results

[11] Figure 1 shows analysed ozone fields on the 26 of February at 0 UT, 26 February at 18 UT and 27 February at 12 UT along with 12 hours of MLS data corresponding to each analysis towards the end of the assimilation experiment. The ozone depletion inside the polar vortex recorded by the MLS instrument is well reproduced in the analysis with minimum ozone values of 850 ppbv. The maximum in ozone above the northern Pacific and the polar vortex tilting are also well represented. Several filamentary structures appear around the edge of the polar vortex. A tongue of polar air is stretching above Europe on the 26 of February at 12 and 18 UT and evolves into a mini-hole above the east Atlantic on the 27 of February. It is not possible to state whether such ozone structures are real features because of the lack of coincidence with supporting data such as MLS or GOME data during this event. Figure 2 reports the time evolution of the zonally averaged assimilated ozone (upper frame) and the forecast error (lower frame). On the first days of assimilation (13 of February onward), the modelled ozone distribution changes very rapidly with lowest ozone mixing ratios at high latitudes and highest mixing ratios at lower latitudes, between 30°N to 60°N, which is opposite to the ozone latitudinal gradient of the ozone climatology used for initialisation. At high latitudes, ozone decreases throughout the assimilation run, reproducing finally the Arctic ozone depletion observed during 1995/1996 winter [*Scientific Assessment of Ozone Depletion*, 1999]. The forecast error decreases from about 35% to 10–20% at middle latitudes and from values greater than 40% to 20–40% at higher latitudes. Figure 3 shows the zonal averages of the OmF, of the OmF RMS, of the forecast error, and of the MLS ozone mean error; the averaging period is from the 26 to the 27 of February. The RMS OmF exhibits a strong latitudinal gradient with an increase from 15% at 40°N to 50% at 70°N. The values of the forecast error are in the same range as the OmF RMS values. The forecast error exhibits a similar, albeit weaker, latitudinal gradient with values ranging between 20% and 30%. The latitudinal variations of the RMS OmF and of the forecast error can be related

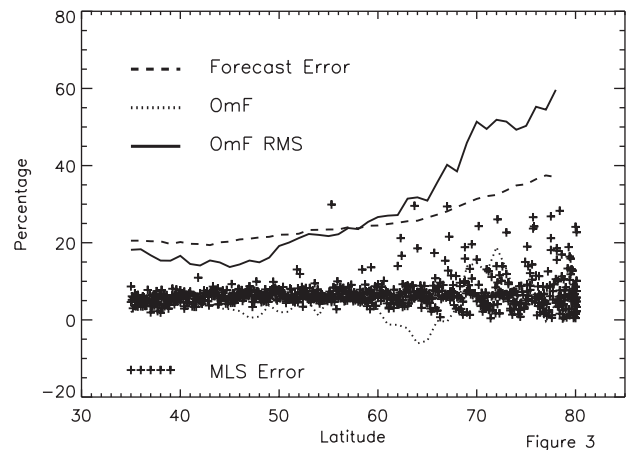


Figure 3. Zonal mean of the forecast error (dashed line), mean OmF (bias, dotted line), the RMS of OmF (solid line), and MLS error (+) as a function of latitude. All the quantities are expressed in percent.

to the higher relative errors of the MLS measurements at high latitudes (see Figure 3). Moreover, a more accurate analysis of the strongly structured ozone field brought about by the polar vortex would require a frequency of sampling much higher than at middle latitudes where the ozone field is relatively flat. Overall, the OmFs do not show any obvious bias although there are some substantial variations at higher latitudes. Previous ozone assimilation studies into CTMs [Khattatov *et al.*, 2000; Levelt *et al.*, 1998], or tracer assimilation with a transport model [Menard and Chang, 2000] found values of forecast error or OmF RMS at higher levels which are lower than the values found here. For example, Levelt *et al.* [1998] found values of the order of 10% at 10 mb. However, the errors increase at lower levels. For the 50 to 20 mbar range, which is more representative of the 550 K isentropic level, Khattatov *et al.* [2000] found RMS OmF values of about 20% to 30%, which is rather consistent with our results.

5. Conclusions

[12] A data assimilation system based on a high horizontal resolution transport model is described. A preliminary evaluation is presented. The use of an isentropic advection model makes the assimilation system well adapted to the assimilation of measurements of long-lived species in the stratosphere. The parametrisation of the forecast error covariance matrix contains a number of simplifications [Menard and Chang, 2000]. Nonetheless, one of the positive features of the parametrisation is the flow-dependency component of the correlation function which is specified according to the PV field. OmF diagnostics indicate that the best analysis are obtained when both distance and PV difference are taken into account in the formulation of the correlation function. The values of adjustable assimilation parameters such as the correlation lengths d_0 or the error growth parameter are found to be of the same order of magnitude as the values obtained in previous studies. The parametrisations of the error covariance leads to a model-calculated variance of the OmF which is in agreement with the uncertainty in the assimilated field derived from the actual observations and the forecast. Chemistry and vertical transport are neglected in this version of the MIMOSA model. Nonetheless, in view of the high sampling frequency of MLS and of the time scales involved, this deficiency should have a marginal effect on the analysis. This is largely supported by the fact that the initial ozone field converges rapidly towards an assimilated field which reproduces most of the structures recorded in the ozone distribution by MLS. However, there are improvements which could be made to the assimilation scheme. For instance, the adjustment of the assimilation parameters is done over the entire model domain. It might be possible to use different values of assimilation parameters at the edge of the polar vortex which is characterised by steep gradients in ozone and PV. The optimal values of assimilation parameters in this region are very likely to be radically different from the middle latitudes or deep inside of the polar vortex where gradients in ozone and PV are relatively weak. The region of the vortex edge can easily be diagnosed from the PV field [Nash *et al.*, 1996]. The model resolution is another potentially important factor for the quality of the analysis which needs to be studied. Finally, we are planning to compare the assimilated ozone with independent high-resolution measurements such as lidar or airborne instruments in order to evaluate further the analysis and investigate the realism of the filamentary structures seen in the assimilated fields.

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