ASSIMILATION OF STRATOSPHERIC OZONE FROM MIPAS IN THE CHEMICAL TRANSPORT MODEL STRATAQ

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ABSTRACT

We use a sequential assimilation approach to assimilate ozone MIPAS profiles into the STRATAQ chemical transport model of the stratosphere. The numerical code uses parameterizations and simplifications allowing assimilation of sparse observations and the simultaneous evaluation of analysis errors. The CTM used is a high resolution three dimensional model which includes a detailed chemical package and is driven by UKMO analysis. Two weeks of MIPAS ozone measurements are assimilated during October 2002, and results validated using data from the SAFIRE-A instrument which is part of the M-55 Geophysica platform operated during the APE-ENVISAT airborne validation campaign.

1. THE CTM MODEL

STRATAQ is a three-dimensional off-line stratospheric chemical transport model that extends from 0.6 km to about 52 km in altitude [1]. The model uses a sigma-pressure vertical coordinate and has a vertical resolution varying from about 11.5 km until 20 km and up to 2.5 km in the higher stratosphere. The horizontal resolution is 5° longitude by 2° latitude. The behaviour of the chemical species is represented by the continuity and transport equation which separately includes the contribution of transport by the large scale circulation and the tendency due to the chemistry. In the CTM chemical species are advected with a semi-lagrangian transport code, using a Van Leer transport scheme that is a monotonic, upstream-biased differencing scheme. Species are transported with a time step of 10 min. Analyzed horizontal wind components, obtained from the United Kingdom Meteorological Office (UKMO), are used to calculate the transport of species. The chemical package includes 43 chemical species, 89 homogeneous gas-phase chemical reactions, relevant to the stratosphere and troposphere, and 33 photolytic reactions. No additional stratospheric-only related detailed chemistry is included in the scheme. To evaluate photodissociation rates J we used a look-up table calculated by a radiative one-dimensional model based on the delta-Eddington approximation. A family approach is employed and a number of short-lived species are combined together into families. The concentrations of species included in the families are calculated assuming photochemical equilibrium conditions. The model uses the semi-implicit symmetric (SIS) method to integrate the chemical continuity equations. A treatment of heterogeneous processes, occurring on the surface of stratospheric background aerosols, NAT (Nitric Acid Tetrahydrate) and ICE particles, is included in the model. The particle surface area density is evaluated without introducing any detailed microphysics. The presence of NAT and ICE PSCs is predicted on the basis of simple thermodynamic considerations, as a function of temperature and HNO3 and H2O local partial pressure, respectively.

2. THE ASSIMILATION SCHEME

A sequential assimilation technique, based on the suboptimal Kalman filter, is used to evaluate the “best” value of the state of the system, or analysis, known prior information [2]. In our case the best estimate of the state of the atmosphere, for instance the atmospheric ozone concentration field, is derived from a linear weighted interpolation of the vector representing the CTM model forecast of the ozone field on the three dimensional grid points, and the vector of observations representing ozone MIPAS profiles along satellite tracks. Operatively, the Kalman filter analysis, once we have fixed a time interval called the “assimilation window” (1 hour) at which the analysis is performed, consists of the following steps:

1. Initialize the model by mean of the chemical constituent concentrations and the error covariance matrix for the ozone field
2. Calculate the updated ozone concentration and error covariance matrix at the beginning of the assimilation window through model integration
3. Collect all observations along the assimilation window (with relative errors) and use them together with the model ozone field as prior information to perform the analysis. Therefore all data over the same window are assumed to be taken at the same time
4. Use then the obtained analysis field as initial condition for the chemistry transport model to predict constituent concentrations at the following time step (i.e.: the beginning of the next assimilation window). Due to the high computational cost of the extended
Fig. 1. Space-time overlapping between MIPAS and SAFIRE-A measurements for the ENVISAT overpass on 24th October 2002 (orbit 3403). Geolocation of individual tangent points (circles) is shown for MIPAS, with tangent heights represented in a false color scale. Location of SAFIRE measurement (stars) is given by tangent latitude and longitude values averaged over each limb sequence. Mean acquisition time for SAFIRE-A scans is also indicated.

Kalman filter approach, some parameterizations have to be introduced. Separate assimilation runs were performed by setting different values of the tuneable parameters. The minimization of OmF bias were used as the base criteria for choosing the best value of the correlation lengths ($L_x=2000$ km and $L_y=0.8$ scale heights). The growth rate of the forecast error ($e=0.02$) and the relative representativeness error factor ($r=0.06$) were calculated to achieve best agreement with observations using the $\chi^2$ diagnostics. The total representativeness error has been parameterized as a function of the vertical levels. In fact, in the assimilation scheme, the whole MIPAS profile is assumed to be taken at fixed latitude and longitude and the horizontal shift between different levels in the same profile is not taken into account.

3. SAFIRE-A DATA

SAFIRE-A (Spectroscopy of the Atmosphere by using Far Infrared Emission - Airborne) [3], is a passive remote-sensor operating aboard the M-55 Geophysica aircraft and capable to perform limb-sounding observations of the atmospheric emission in the far-infrared region, in narrow spectral bands ($\approx 2$ cm$^{-1}$) between 20 and 200 cm$^{-1}$, with a spectral resolution of 0.004 cm$^{-1}$ unapodized. Sequences of individual spectra acquired at different limb angles are processed to retrieve the VMR (Volume Mixing Ratio) vertical profiles of minor atmospheric constituents. During the 2002-2003 ENVISAT validation campaigns with the M-55, the instrument configuration was set for measurements of O$_3$, HNO$_3$, N$_2$O, ClO, H$_2$O and HCl. Measurements of O$_3$ acquired by SAFIRE-A during the mid-latitude validation flight on the 24th October 2002, in coincidence with an overpass of the ENVISAT satellite (orbit 3403), are used as independent data set to validate the CTM analysis results. During the chosen flight, SAFIRE-A acquired 20 limb scanning sequences, obtaining several profiles of the target species at approximately the same time and with reasonably co-located with MIPAS measurements (see Fig. 1).

4. THE SIMULATION

The sequential assimilation algorithm, coupled with the three dimensional chemical transport model, has been used to assimilate MIPAS ozone observations for a test
Fig. 2. Time and zonally averaged OmF (MIPAS minus forecast) mean difference. The temporal mean is calculated over the whole assimilation period.

Fig. 3. Plot of $\chi^2/N$ as a function of time for the whole assimilation period. Each value is computed for one assimilation analysis.
two week period during autumn 2002. The simulation has been performed to reproduce the atmospheric chemical situation relative to the end of October 2002 due to the availability, during this period, of SAFIRE-A data. For the simulation the model has been initialized using output fields from long-term integration performed with a low resolution CTM relative to October of a previous year. Two weeks of free model integration has been then performed to reproduce the chemical-dynamical situation relative to 10th October 2002. MIPAS data have been then assimilated for the following two weeks until October 24th. An initial background error of 10% was fixed for the ozone field.

5. RESULTS

Fig. 2 presents the time and zonally averaged difference between observations and first guess forecast (OmF). OmF bias has been minimized to set the correlation lengths of the forecast errors. This bias reflects data accuracy and precision and, at the same time, it is a measure of the forecast skill. The bias shows absolute values lower than 30%. It is usually below 10% around 35 km and it grows above and below this region in correspondence to a decrease of accuracy of MIPAS data. High values above about 45 km seem to be also related to known presence of a model bias on the fast photochemistry. Other parameters of the system where fixed to allow the value of $\chi^2/N$, where $N$ is the number of observations used in the assimilation analysis, to tend to unity and not exhibit a temporal trend. The $\chi^2/N$ time behavior over the assimilation period is shown in Fig. 3.

Fig. 4 shows analyzed ozone fields for 24th October 2002 22 UTC, zoomed over southern Europe. The map is relative to the 67 hPa level corresponding to about 20 km, which is the maximum M-55 flight altitude for the chosen day. The resulting analysis field works as an extension of MIPAS satellite data, originally sparse and scattered in time and space on the whole globe, to a regular grid for the selected time, and shows noticeable latitudinal gradients in the zone sampled by SAFIRE-A. For comparison purpose the resulting CTM field is time-space interpolated onto SAFIRE-A tangent points and resulting profiles then compared to the original SAFIRE-A retrievals.

Fig. 4. False color map of $O_3$ mixing ratio at about 70 hPa, on 24th October 2002 resulting from the assimilation of two weeks of MIPAS ozone measurements. Values are in ppmv. Results are shown over Europe at 22:00 UTC.
Fig. 5. Comparison between O₃ profiles obtained by SAFIRE-A during the M-55 GEOPHYSICA validation flight of 24th October 2002 (20 scans obtained from about 19 to 22 UTC over central Italy) and CTM assimilated O₃ field for 22 UTC interpolated on the positions of SAFIRE-A retrievals. Data for MIPAS (scan 15 orbit 3403) are also shown in the selected altitude range.

Fig. 6. CTM assimilated MIPAS O₃ versus SAFIRE-A O₃. Assimilated field is interpolated on the positions of SAFIRE-A retrievals, as in the precedent figure. Tangent heights of the data points is represented in a false color scale.
Results are shown in Fig. 5, together with the MIPAS overpass data, highlighting a substantially fair agreement between the data sets (note the possibility of performing a SAFIRE-A to MIPAS assimilation comparison also below the lower tangent altitude sampled by the chosen overpass). CTM interpolated data show less variability than SAFIRE-A retrievals on a constant pressure level, due to the relative low horizontal resolution of the model grid. The spread of the VMR distribution measured by SAFIRE-A over the sampled region (that can be considered in close proximity with the location of MIPAS measurements) is not surprising and should be related to the presence of the strong O₃ horizontal gradient shown even by the CTM field in the zone of measurement. From the analysis of the scatter plot shown in Fig. 6, CTM assimilated MIPAS O₃ appears to show an overall good correlation with SAFIRE-A O₃.

REFERENCES
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