THE PROMOTE OZONE PROFILE SERVICE – LONG-TERM 3D OZONE REANALYSIS OF ERS-2 AND ENIVSAT DATA SETS

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ABSTRACT

The service aims at providing a global reanalysis of ozone and related conservative and reactive species in the stratosphere by exploiting observations from ERS-2/GOME, ENVISAT/MIPAS, SCIAMACHY and GOMOS as well as UARS/MLS. The target period covers the years 1992 to present will be covered. In order to derive a global consistent record of stratospheric ozone chemistry an ensemble of data assimilation systems is applied. This suite comprises a Suboptimal Kalman-Filter (KF) using ROSE/DLR and four-dimensional assimilation (4D-Var) systems SACADA and BASCOE. The service is part of the GSE PROMOTE portfolio. PROMOTE is the GMES Service Element (GSE) for the Atmosphere (http://www.gse-promote.org). Reanalysis results are presented as well as first applications on the evaluation of coupled chemistry-climate models.

1 INTRODUCTION

The state of the earth's ozone layer and its future trend has serious implications on the biosphere and climate. Therefore, a continuous monitoring of the ozone layer and a better understanding of stratospheric processes related to ozone depletion is crucial for organizations like SPARC (Stratospheric Processes And their Role in Climate) and WMO (World Meteorological Organization). While satellite and ground-based measurements are used for monitoring the ozone layer, coupled-chemistry climate models (CCMs) are applied to provide ozone predictions for the WMO/UNEP and IPCC assessments [21,17].

In order for their results to be credible and treated with confidence, CCMs must be carefully validated against measurements and other models. The GMES (Global Monitoring of Environment and Security) PROMOTE ozone record will contribute in fulfilling the general objective to better evaluate the three-dimensional representation of ozone in coupled chemistry-climate models [14]. Therefore, the CCMVal Activity for SPARC (http://www.pa.op.dlr.de/CCMVal) joined PROMOTE as core user for the ozone profile service.

In response to the users' needs, DLR and BIRA-IASB build a joint service based on the satellite-based chemical observations from ERS-2, ENVISAT and UARS to derive a long-term three-dimensional ozone record and additional information on ozone related species. It aims at analysing catalytic ozone depletion in gas phase and on aerosols and investigating the stratospheric budget of inorganic reservoir species.

In recent years DLR and BIRA-IASB have both developed demonstration services to derive stratospheric ozone analyses on a routine basis [8, 11, 15]. Since the combination of physico-chemical models and satellite observations via data assimilation can give a consistent description of the atmosphere's state, it additionally allows for the analyses of processes that drive ozone chemistry and dynamics [4, 18].

This conjoint service, consisting of the Kalman-Filter data assimilation system ROSE/DLR and the 4D-Var assimilation systems BASCOE (Belgian Assimilation System for Chemical Observations from ENVISAT) [13, 15] and SACADA (Synoptic Analyses of Chemical Constituents by Advanced Data Assimilation) [6, 20], will provide an ensemble of two long-term complementary data sets from 1992 to present.

To ensure high quality of data products, validation and evaluation work is an integral part of this service. Collaboration with research partners is foreseen to foster the discussion of scientific issues related to data assimilation and remote sensing.

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2 DATA ASSIMILATION SYSTEMS

The service will make use of three different data assimilation systems:

- ROSE/KF: suboptimal Kalman-Filter based sequential assimilation providing analyses and error estimates (to improve 4D-Var)
- SACADA: four-dimensional variational assimilation using error estimates from ROSE/KF
- BASCOE: four-dimensional variational assimilation

The following base parameters will be delivered as global synoptic analyses with 24h and 6h temporal resolution:

- Reactive ozone chemistry: O3, O3-depletion rates, ClOx, NOx and PSCs
- Inorganic reservoir species: Cly

The assimilated data record will cover the time periods 1992 until 1999 (BASCOE/MLS), 2002 until 2004 (BASCOE/MIPAS) and 1995 (DLR) until now depending on above listed observations. The service will be extended at least to the ENVISAT instrument live time.

2.1 Suboptimal Kalman-Filter/ROSE

A suboptimal Kalman-Filter in conjunction with the stratospheric chemistry-transport model ROSE/DLR is applied for sequential assimilation of ERS-2/GOME and ENVISAT/MIPAS trace gas observations [1]. Thereby a continuous global vertical resolved ozone record is generated covering the years 1995 until 2005. The data assimilation scheme is optimum interpolation (OI) based with KF-like covariance diagnostics. The method is fast, allowing the derivation of background covariances by repeated analysis cycles. Optimized assimilation parameters are derived using χ^2 diagnostics. Derived products consist also of first-guess minus observation (FMO) error statistics. Results will serve as a first quality check for observations and model calculations. Error estimates will be applied to improve the covariance parameterization in 4D-Var SACADA (see **Fehler! Verweisquelle konnte nicht gefunden werden.**).

Released products will consist of synoptic ozone maps (with ozone analysis errors), chemical ozone loss rates and area densities of NAT – ICE PSCs [16].

2.2 Four-dimensional Assimilation

The 4D-Var method aims to optimize the model initial condition to reproduce a set of observations given for a time window [12]. One of the benefits of this method is that it creates a balance analysis throughout the assimilation window. For example to reproduce ozone data, initial condition of every species that interact significantly with ozone during the time window will be adjusted. This method can then derive information from unobserved species like chlorines.

2.2.1 SACADA System

4D-Var assimilation of observed atmospheric chemical constituents allows for chemically consistent analyses of the current state for a certain time and location. The SACADA system was developed from the stratospheric general circulation model COMMA and the meteorological forecast model GME [6, 16, 20]. It utilizes a numerically efficient icosahedron spherical grid structure. Thus, SACADA scales well on medium sized PC clusters. At DLR, SACADA was adapted for continuous long-term applications for synergistic use of data from various atmospheric instruments. To improve SACADA covariance parameterization error estimates from the ROSE ozone products service (see 2.1) will be used to derive variable length scales depending on atmospheric conditions. The Rhenish Institute for Environmental Science RIU) is closely involved as research partner to improve the model systems' chemistry module.

SACADA ozone products will focus on reactive ozone chemistry. Besides providing global ozone mixing ratios, analyses of chlorine and nitric oxides will be derived globally for fixed local times. Due to considerable computing demand, the service will initially process the more recent 2002 – to date period (better instrumental coverage) and then reprocess older dates back to 1995.

Released products will consist of synoptic ozone maps and asynoptic maps of ClOx and NOx for fixed local times.

2.2.2 BASCOE System

The Belgian Assimilation System for Chemical Observations from ENVISAT (BASCOE) is a 4D-Var assimilation scheme [13, 15]. It has been applied operationally to near real time MIPAS observations: O3, NO2, HNO3, N2O, H2O and CH4 (see http://bascoe.oma.be).

For this service, BASCOE analysis of MIPAS and UARS/MLS will be provided as synoptic maps. This concerns ozone and chlorine reservoir Cly.

3 DATA

The PROMOTE ozone profile record service will mainly exploit data of the European instruments ERS2/GOME, ENVISAT/MIPAS, SCIAMACHY and

GOMOS. This data will be complemented by NASA/ UARS and AURA/MLS. Application of MetOp/GOME-2 and IASI instruments is envisaged but depends on data quality and availability. For scientific purposes, also data of the Canadian ACE/FTS instrument will be used. Other observational data from TOMS, HALOE and ground-based observations are applied for accompanying validation purposes.

Data is received by the standard ESA data distribution service for operational data products. The research partner Service d'Aeronomie will provide additional GOMOS data on NOx and ozone. Additional MIPAS chemical observations are obtained from IMK/FZ Karlsruhe.

GOME ozone profiles from the ESA-CHEOPS project are used which have been retrieved by the NNORSY approach [19, 7].

4 FIRST RESULTS

In the following we briefly present latest results of the ROSE/KF data assimilation system. For most recent results on BASCOE we refer to [13] within this proceedings. For latest results on SACADA please see [20].

4.1 Assimilation of MIPAS data

Due to different retrieval schemes available MIPAS chemical observations from 2002 to 2004 differ in quality and coverage. Therefore, we have investigated the sensitivity of the data assimilation scheme (chapter 2.1) to two different sample data sets [1]. ENVISAT/MIPAS baseline observations of H2O, O3, HNO3, CH4, N2O and NO2 from the ESA operational product and the IMK (Institute for Meteorology Karlsruhe) scientific product are considered.

It is shown that all assimilated model species benefit significantly from observations. Results are analyzed using observation minus forecast error (OmF) statistics. In order to strengthen the consistency of the analysis, results of a χ^2 diagnostics were employed to improve the initial background and representativeness errors. Due to strong scatter with altitude and latitude the corrections are found especially significant for MIPAS/ESA data. Improvements to model results without assimilation of MIPAS data were quantified by comparisons to HALOE observations. Results show an r.m.s. error reduction of up to 30% for the assimilated species. The positive influence of data assimilation is also found in the analysis error which significantly decreases where observations are available.

Although assimilation of MIPAS/IMK data performs in general better compared to the respective MIPAS/ESA experiment, the mean assimilation results are comparable with some exceptions: assimilation of MIPAS/IMK data leads in particular to higher H2O mixing ratios in the lowermost stratosphere. Two regions with increased H2O values near the tropical tropopause, covered both by MIPAS/ESA and MIPAS/IMK data, show only up in the results with MIPAS/IMK data. Despite the differences it has to be emphasized that MIPAS/ESA data has been processed within an operational environment and shows in general better temporal coverage.

In summary, both MIPAS/IMK and MIPAS/ESA data

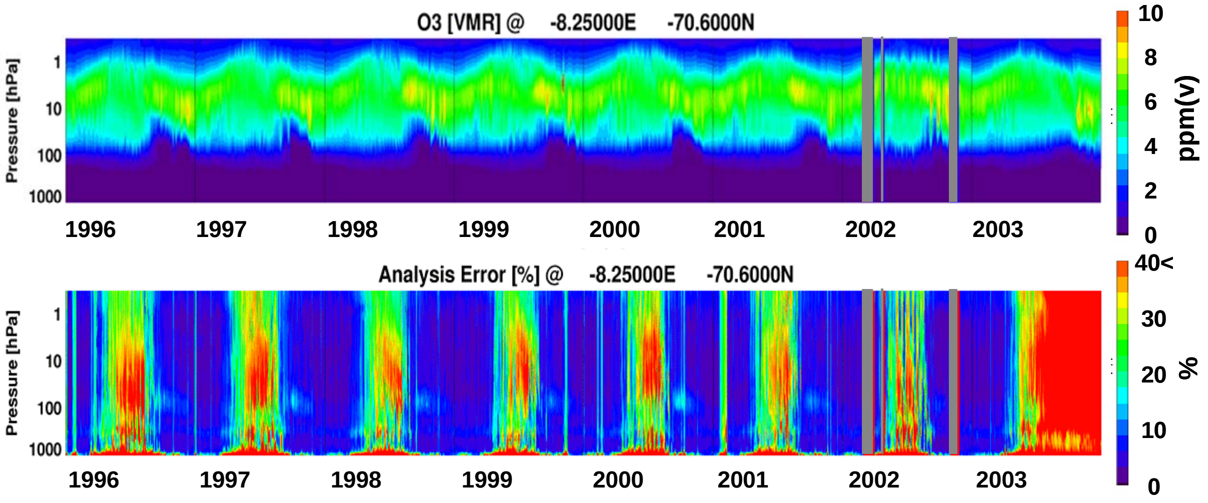

Figure 1: Assimilated stratospheric ozone record as derived from GOME/NNORSY observations from 1996 to 2003. A time series of ozone volume mixing ratios in ppm(v) over Neumayer, Antartica is depicted. Below the corresponding analysis error in percent is shown.

sets are found to be well suited for global chemical data assimilation, while overall analysis errors are smaller when MIPAS/IMK data is used.

4.2 Assimilation of GOME/NNORSY data

By means of assimilating all GOME/NNORSY ozone profile observations from 1996 to 2003 a highly consistent and complete global 3D record of ozone volume mixing ratios is now available (Fig.1) [7, 9]. About $50x10^6$ ozone profiles have been assimilated by the sequential Kalman-Filter based approach (chapter 2.1) using the chemical-transport model ROSE/DLR 3.0 [1]. In a validation study based on LIDAR measurements at different latitudes GOME/NNORSY ozone profiles showed the smallest rms error (<10%) and the lowest bias compared to Optimal Estimation and Phillips-Tikhonov approaches [19]. As an example Figure 1 presents a time series of ozone mixing ratios over Neumayer, Antarctica from 1996 to 2003. The seasonal variation of ozone is clearly visible. Each September and October massive ozone destruction within the undisturbed polar vortex results in low mixing ratios from 100 hPa to 30 hPa. Due to a very early mayor final warming on September 25, 2002 the ozone depletion is weaker in that year.

Beside the ozone reanalysis a global error statistics has been derived based on quantities like observation minus forecast error (OmF), observation minus analysis error (OmA) or the analysis error [7, 9]. The OmF and OmA errors of GOME/NNORSY version 3-0 prove in general a very smooth behavior and never exceed 0.6 to -0.2 ppmv except for the terminator regions. Time series of zonal mean OmF and OmA errors for several pressure levels confirm these findings.

Results of the analysis error reveal an estimate of the general reliability of the reanalysis data (Figure 1, bottom). This is important auxiliary information for any further use of the data. When GOME/NNORSY observations are present, the analysis error is always below 25% and in most cases below 10%. Thus, the analysis reaches a high level of reliability.

The assimilated ozone record is compared directly to statistical moments based on the observational data only. In case of zonal means the data sets differ below 4% for the largest part of the stratosphere. Analysis and observations further deviate to a larger extent around the tropopause. However, this region of high dynamical variability is in general difficult to examine. Results from the geophysical validation will help to interpret these deviations.

In order to give an independent estimate on the quality of the assimilated ozone record, comparisons to HALOE chemical observations have been conducted. We apply HALOE version 19 data available from January, 1996 until April, 2003 (see http://haloedata.larc.nasa.gov) for sunrise and sunset conditions. Observations are limited to latitudes between 70°S and 70°N. HALOE measures about 20 ozone profiles per day. The known accuracy of a single observation is better then 15% within the stratosphere. Only data above the tropopause (defined by 2 potential vorticity units [10-6K m² /kg /s]) is considered.

In most cases the reanalysis and HALOE observations agree within 10%. Bias is in general smaller than +/- 3%. During the course of each year analyzed a weak positive trend in mean errors is visible.

4.3 Comparison to E39/C

To demonstrate a first application of this PROMOTE service Figure 2 depicts monthly mean ozone mixing ratios from assimilated GOME/NNORSY data (2a) [7] and as calculated by the CCM E39/C (2b) [3]. Results from 1996 to 1999 for 100 hPa, 50 hPa, 30 hPa and 10 hPa (from top) are shown. It can be seen that E39/C captures the variability mainly well. Differences occur at high latitudes e.g. the inter-annual variation of the ozone hole is underestimated. On the contrary, E39/C exceeds the variability in northern high latitudes. A positive bias in E39/C is evident at 50 hPa, while a negative one can be detected at 30 hPa.

Beside a comparison of statistical moments the ozone profile record will also for more process-oriented studies like chemical ozone-loss or denitrification. Also hemispheric quantities related to dynamics and chemistry are of interest [10]. In the near future studies will be extended to a larger number of models participating in the SPARC CCMVal activity [14].

5 SUMMARY AND OUTLOOK

In order to derive the best affordable description of the chemical state of the stratosphere, satellite data from ERS-2, ENVISAT and UARS/MLS, meteorological data and chemistry-transport modeling is synergistically combined by means of data assimilation. The focus is on synoptic 3D ozone analyses and long-term analyses of trends in reactive trace gases and inorganic reservoir species. The envisaged period is 1992 to present.

A first assimilated ozone record is available from 1996 to 2003 using GOME/NNORSY ozone profile observations. The record shows low OmF errors and a good agreement with collocated HALOE observations (rms <10%). An assimilated record using MPAS/ROSE

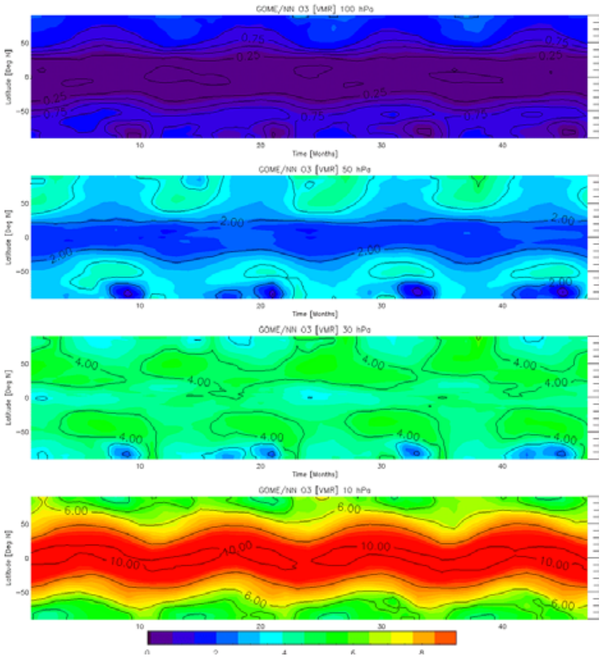

Figure 2a: Ozone volume mixing ratios at different pressure levels (100, 50, 30 and 10 hPa) from GOME/NNORSY reanalysis (1996 to1999).

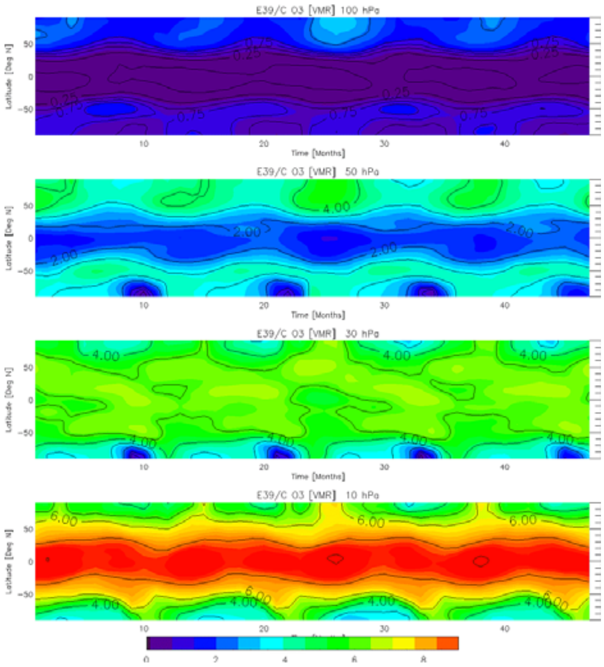

Figure 2b: Ozone volume mixing ratios at different pressure levels (100, 50, 30 and 10 hPa) from the CCM E39/C (1996 to 1999)

MIPAS/ROSE/KF from 2002 to 2004 exhibits a fairly good agreement with chemical observations from HA - LOE, too. Based on BASCOE a reanalysis of 18 months of MIPAS and 4,5 months of GOMOS was performed [13]. For O3 and NO2 this study reveals a good agreement between the two sets of analyses, which suggests a good agreement of the two instruments. Finally, some data assimilation experiments were carried out comparing analyses of MIPAS data by the 4D-Var data assimilation system SACADA and a suboptimal Kalman-Filter approach. It can be concluded that the 4D-Var scheme delivers in general better results on chemical constituents.

The next steps are to assimilate UARS/MLS with BASCOE and GOME/MIPAS/GOMOS with SACADA. For the latter the GOME/NNORSY/ROSE record will be used for initialization.

To reach the final objective a continued comparison with ground-based and satellite-based observations is necessary. Of special focus is the evaluation of overlapping periods (e.g. 2002/2003) with respect to consistency. Here long-term observations from MLS and HALOE will be considered. Once the final stratospheric record of ozone and related species is assembled, comparisons to CCMs together with the user SPARC CCMVal will be made.

The resulting ozone profile record will be available as quick-looks, HDF4 and NetCDF files via the PROMOTE web site (http://www.gse-promote.org).

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