SCIAMACHY OZONE COLUMN VALIDATION WITH MODELS AND ASSIMILATION

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ABSTRACT

In this paper we report the results of three validation studies. First, a comparison of the recently processed SCIAMACHY "validation reference set" ozone columns (software version 5.01) with assimilated ozone fields based on the new GOME ozone column retrieval of KNMI (TOGOMI). Second, a direct comparison between the SCIAMACHY "validation reference set" and the scientific retrieval of the KNMI (TOSOMI) algorithm. Third, a monitoring of the early 2004 SCIAMACHY total ozone meteo product with the ozone analyses of the ECMWF model. The SCIAMACHY operational ozone column product has improved compared to ACVE-1, but an upgrade of the processor is still urgently needed to include the latest algorithm developments implemented for the GOME ozone column retrieval. The TOSOMI scientifically retrieved O3 column of KNMI is a stable product with a small bias < 1% compared to GOME-TOGOMI and an overall bias of −1.5% compared to Brewer and Dobson. The SCIAMACHY operational ozone data showed large problems in March and April 2003.

1. INTRODUCTION

Data assimilation complements validation with independent observations. The differences between the model forecast and new observations that have not been used in the assimilation (the observation minus forecast departures, OMF) provide a wealth of information about the model performance, the quality of the observations and the retrieval approach. These departures form the core of each data assimilation system: all new observation are first compared with a model prediction of this observation. Based on the OMF departures and knowledge of the observation and forecast error statistics, the model state is updated in the assimilation step to account for the information brought by the observations. With the forecast model one can construct a model predicted value for each of the typically millions of satellite observations available, and statements can be made with great statistical confidence. This is an advantage compared to validation studies with ground stations and balloon and aircraft campaigns, where only typically between one and a few hundred collocations are available. The forecast, however, is itself based on earlier observations of the same, or similar, satellite sensors. Therefore assimilation of one data set alone can not fully determine the quality of the satellite observations, for which independent observations are crucial.

In this contribution we will discuss the use of ozone data assimilation models to learn about the quality of the SCIAMACHY near-real time (NRT) total column ozone product and the results of the scientific DOAS ozone retrieval algorithm of KNMI, called TOSOMI. This paper discusses three validation studies:
(i) Monitoring of the SCIAMACHY operational ozone column product of ESA and the TOSOMI scientific product of KNMI for the SCIAMACHY validation reference set (SVRS).
(ii) A direct comparison between the two retrievals.
(iii) A monitoring of the same two ozone retrievals with the ECMWF IFS assimilation model for the period January-April 2004.

For data assimilation a continuous and global data set without large data gaps would be ideal. Unfortunately the availability of SCIAMACHY NRT ozone column data processed with the latest version 5.01 of the processor has been sparse (see, e.g. figure 1 for a geographical overview of the states availability for validation). In this paper we will focus on the period August - October 2002. Since the limited coverage does not allow for an assimilation of the data we have monitored the available NRT data against assimilated GOME ozone fields.

Figure 1. Coverage of the Sciamachy validation reference set, August-October 2002. Shown are the mean SCIAMACHY total ozone values during this period, gridded on a 2x3 degree grid.
2. SCIAMACHY DATA SETS

2.1 ESA near-real time operational processor

The SCIAMACHY processor is described in the Algorithm Theoretical Basis Document available on the ESA-ENVISAT web site [SCIAMACHY 2000]. The ozone column is retrieved from the SCIAMACHY measurements based on the DOAS technique [Bovensmann 1999], and the current versions of the software are based on the GOME data processor GDP v2.x. During the first ACVE meeting several shortcomings have been identified with earlier versions 3.51, 3.52, 3.53 of the near-real time (SCI_ARC) total ozone products from SCIAMACHY [Lambert 2003; Eskes 2003b; Meirink 2003].

In early 2004, the SCIAMACHY NRT processor was upgraded to the newly operational version 5.01. The results presented in this paper will be based on this new processor and on the latest operational data sets of early 2004. In preparation of the ACVE-2 meeting ESA has processed about 1900 SCIAMACHY states and these states were made available to the validation teams in March 2004. This was a subset of the 2591 states defined by the validation teams, the so-called "validation reference data set". The set of states is limited to the period from July to November 2002 and does not allow for a study of the seasonal dependence of the data products.

2.2 TOSOMI Scientific Processor

The KNMI SCIAMACHY total ozone retrieval algorithm (TOSOMI, current version 0.31, November 2003) is an application of the TOGOMI algorithm to SCIAMACHY. The new GOME algorithm TOGOMI [Valks 2003] is based on the total ozone DOAS (Differential Optical Absorption Spectroscopy) algorithm developed for the OMI instrument [Veefkind 2001]. With respect to total ozone column retrieval using the DOAS method, the OMI, SCIAMACHY and GOME instruments are very similar. The main improvements of the new algorithm are:

(i) treatment of the atmospheric temperature sensitivity by using effective ozone cross-sections calculated from ECMWF temperature profiles,
(ii) improvements in the calculation of the air mass factor, using the so-called empirical approach,
(iii) using the Fast Retrieval Scheme for Clouds from the Oxygen A-band (FRESCO) algorithm for the cloud correction,
(iv) a new treatment of Raman scattering in DOAS [De Haan 2003]. This new formulation of DOAS explicitly accounts for the smearing of the solar Fraunhofer lines as well as the atmospheric tracer absorption structures, and
(v) air-mass factors based on semi-spherical polarization-dependent radiative transfer (KNMI DAK model).

The SCIAMACHY total ozone retrieval algorithm TOSOMI combines a Sciamachy level-1 product reading module with the TOGOMI DOAS modules. The Fresco algorithm [Koelmeijer 2001] is applied to the Sciamachy spectra to obtain cloud fraction and cloud top height estimates.

3. MODELS AND ASSIMILATION

The NRT SCIAMACHY ozone column data and the scientific TOSOMI ozone columns have been monitored with the KNMI ozone column assimilation scheme TM3DAM and the operational ozone analyses of ECMWF.

3.1 The tm3dam ozone data assimilation system

The assimilation model TM3DAM (TM3 Data Assimilation Model) is described in detail in Eskes et al. [2003a]. The transport model is based on the second moment advection scheme and has 44 vertical levels and is run with a resolution of 3x2 degree. The model is driven by the meteorological analyses of the European Centre for Medium-Range Weather Forecasts. Stratospheric ozone chemistry is described by two parametrisations, one for gas-phase chemistry and one for heterogeneous ozone loss in the polar regions. The assimilation uses a fast parameterised Kalman filter approach which provides ozone analyses.
and detailed forecast error estimates. Both OMF and observation-minus analysis data sets are routinely provided.

The model assimilates KNMI TOSOMI near-real time ozone columns derived from the SCIAMACHY measurements. The data base of ozone analyses and daily ozone forecast are made available via the TEMIS web site [TEMIS].

For the validation of the SCIAMACHY validation reference set which has become available early 2004 we have performed a separate assimilation run for August-October 2002. This is based on GOME ozone columns retrieved with the new TOGOMI DOAS ozone column retrieval code [Valks 2003]. TOGOMI and TOSOMI are both based on the OMI-DOAS algorithm [Veefkind 2001]. They differ only in their specific application to GOME or SCIAMACHY measurements respectively.

### 3.2 ECMWF ozone analyses

Ozone is fully integrated into the ECMWF forecast model and analysis system as an additional three-dimensional model and analysis variable similar to humidity. The forecast model includes a prognostic equation for the ozone mass mixing ratio. Ozone chemistry is described by a parametrisation which is an updated version of Cariolle and Dèqué. Ozone data assimilation is performed in the operational ECMWF 4D–VAR assimilation system and also in the 40-year reanalysis project (see [Dethof 2002] for more details). The operational implementation is based on SBUV-2 ozone columns and stratospheric profiles, GOME ozone columns (until June 2003), and, more recently, on MIPAS NRT ozone profiles [Dethof 2004]. ECMWF is actively participating in the validation activities for ENVISAT.

### 4. SCIAMACHY VS ASSIMILATED GOME

Figure 1 shows the geographical distribution of the SVRS. In this section we present results of the comparison of the SCIA_NL version 5.01 processed at these locations and the TM3DAM assimilated total ozone analyses based on the GOME-TOGOMI retrievals. For comparison we also show the TOSOMI ozone columns retrieved for the same SVRS.

In figure 3 we show the latitude dependence of the comparison. In the Northern Hemisphere over Europe there are a reasonable amount of reference states available for meaningful conclusions.

The operational retrieval, SCIAMACHY NRT, show a bias which, on average is smaller than 1% compared to the assimilated GOME-TOGOMI results. This result is in contrast to the large negative bias reported during the first ACVE of December 2002, and demonstrates an improvement over the previous versions of the operational ozone column product.
The bottom figure shows that GOME-TOGOMI and SCIAMACHY-TOSOMI retrievals have a very small average relative bias (< 1%). Since the underlying algorithms are identical, this result shows that calibration aspects (e.g., radiometric calibration) do not substantially influence the ozone column DOAS retrieval in the 325-335 nm window. The fit residuals of the TOSOMI and TOGOMI retrievals are both small, of the order of 0.5%. It is important to note that the monthly-mean latitude-dependent bias between the model forecasts and the TOGOMI data that is assimilated is generally < 1%, and the global average bias is negligible. Latitude-longitude plots of the bias seem to show a better consistence (less scatter) for TOSOMI than for SCIAMACHY NRT when compared with the assimilated model fields.

In the Southern Hemisphere it is more difficult to draw conclusions because of a more sparse distribution of the reference states. For instance the positive bias observed between 30-40S is related to a single state west of South Africa, and is not statistically meaningful. The comparison is further complicated by strong gradients related to the ozone hole, the anomalous splitting of this ozone hole in 2002, the large solar zenith angles and possibly biases introduced by the model (due to values transported from the unobserved dark winter pole). More data is definitely needed to arrive at conclusions.

Figure 4 shows the OMF difference for the SCIAMACHY operational ozone columns. This shows an increase in ozone from East to West viewing pixels of about 2%. On top of this there is a difference between backscan and forward scan pixels: the backscan is higher for the East pixels and lower for the West pixels. Similar plots were made for the TOSOMI which shows very little viewing-angle dependence. However, the backscan - forward scan asymmetry is also observed in the TOSOMI data set. A possible reason for this is a small error in the geolocation parameters in the level-1 files.

Figure 5 shows the OMF difference for the SCIAMACHY operational ozone columns. This shows an increase in ozone from East to West viewing pixels of about 2%. On top of this there is a difference between backscan and forward scan pixels: the backscan is higher for the East pixels and lower for the West pixels. Similar plots were made for the TOSOMI which shows very little viewing-angle dependence. However, the backscan - forward scan asymmetry is also observed in the TOSOMI data set. A possible reason for this is a small error in the geolocation parameters in the level-1 files.

Figure 5 shows that the operational and TOSOMI retrievals both have a significant cloud-fraction dependence. For the SCIAMACHY NRT product the ozone amount increases by 2-3% when the cloud fraction increase from 0 to 1. The TOSOMI retrieval increase by 1-1.5% from 0 to 0.9 cloud fraction. Cloud fraction 1 is exceptional, with 1.5 to 2% higher ozone and a high population compared to OCRA. This suggests that at least part of the cloud fraction dependence is related to peculiarities of the FRESCO scheme (see also the paper by Fournier [2004]).

5. SCIAMACHY NRT VS TOSOMI

For the direct comparison of the operational SCIAMACHY ozone product and the TOSOMI scientific product we have applied the TOSOMI algorithm to the updated level-1 data of the SCIAMACHY validation reference set (SVRS) that became available early 2004. The two level-2 products were compared on a 1 to 1 basis.

Figure 6 shows the direct comparison of the ozone values for the northern hemisphere, tropics and southern hemisphere mid-latitudes (top panel). There is a good correspondence between the retrievals, with a mean agreement better than 15 DU for all ozone values (mean bias 0.5%) and a standard deviation of 6 DU (about 2%).

The South Pole shows a different behaviour, with large differences for the larger ozone values. Above 350 DU the two retrievals start to deviate. The SCIA_NL product reaches higher ozone levels of around 400 DU, whereas the higher ozone values of TOSOMI reach up to 500 DU. We note that these high values are exceptional and are related to the split ozone hole conditions. These values occur close to the pole with high solar zenith angles.

Figure 7 shows the comparison as a function of latitude. Between 50S and 50N the bias between the two products is within 4%. For larger latitudes (and solar zenith angles) the difference becomes larger, especially in the southern hemisphere.

Figure 8 looks at the intermediate DOAS result, namely the slant column. This is directly related to the depth of
the absorption features and is related to the amount of ozone along the path the light travels through the atmosphere. The figure shows striking differences. Two important aspects to explain the differences are the different treatment of rotational Raman scattering [de Haan 2003] which causes TOSOMI to be higher than SCIAMACHY NRT by 2-3% (low latitudes) to 7-9% (high latitudes). A second important aspects is the difference in cross-sections used (SCIAMACHY-FM versus GOME-FM) which causes TOSOMI to be lower than SCIAMACHY NRT by about 6%. Especially the large impact of the rotational Raman effect demonstrates the need for an urgent upgrade of the SCIAMACHY processor to a DOAS scheme that accounts for this.

6. OZONE MONITORING AT ECMWF

ENVISAT retrieval products are routinely monitored and/or assimilated with the ECMWF operational model. These include:
(i) ESAS SCIAMACHY operational total column ozone meteo product, monitored at ECMWF since February 2003, and
(ii) KNMIS TOSOMI NRT total column ozone data, monitored at ECMWF since 21 March 2004.
the mean departure with the ECMWF model is about 20 DU. At least part of this 20 DU will be related to the ECMWF analyses, which is currently assimilating only a limited set of ozone data, consisting of SBUV columns and stratospheric profiles. Both ENVISAT MIPAS ozone profiles and GOME ozone column data are no longer available in this month (on a global scale).

The problems with the meteo products have in the mean time been identified and corrected.

7. CONCLUSIONS AND PERSPECTIVES

The main conclusions for the three inter-comparisons presented in this contribution are:

**Sciamachy vs assimilated GOME-TGOMI**

The reprocessed SCIAMACHY operational data set, and the TOSOMI scientific product have been compared with assimilated GOME TOGOMI ozone fields. This was done for the validation reference set, for the period August-October 2002. The main results are:

- The overall bias between (assimilated) GOME TOGOMI, SCIAMACHY-operational and TOSOMI is small, < 1%. This is a clear improvement compared to the status of the operational products reported at the first ACVE.
- The TOSOMI product is about 1.5% lower than Brewer and Dobson measurements.
- The standard deviation of TOSOMI and SCIAMACHY NRT minus assimilated GOME is about 3%. This is a good result, demonstrating that the noise in both products is low.
- A viewing angle dependence was detected in the NRT product of about 2% difference between East and West.
- A cloud fraction dependence is found in both the TOSOMI and SCIAMACHY-NL products. There is a 2 - 2.5% ozone difference between cloud fraction 0 and cloud fraction 1. For the TOSOMI product the pixels with cloud fraction = 1 are anomalous, which may be related to the FRESCO cloud retrieval scheme.
- The validation reference set is too limited for validation based on data assimilation: full coverage is needed for more detailed studies.

**Sciamachy ozone monitoring at ECMWF**

The operational SCIAMACHY meteo product and the KNMI TOSOMI ozone columns have been monitored with the ECMWF model. The main results are:

- The ESA product is normally relatively stable, but there were large jumps observed in ozone (order 40 DU) in March and April 2004.
- A negative bias (−30 DU) is found in the comparison between the SCIAMACHY meteo data and the ECMWF
model ozone. This bias got worse after 28 March 2004 (values of 60 DU in global mean).

- The TOSOMI product agrees better with the ECMWF ozone analyses than the SCIAMACHY NRT product (−20 DU difference).
- A data gap exists between about 90-150E. Data from ftp-pde.envisat.esa.in is not available in NRT and comes too late for analysis.
- Geolocation information (e.g. FOV, SZA) is still not included in the SCIAMACHY meteo data product, despite repeated requests.
- The stability and NRT delivery of the SCIAMACHY meteo product is currently not good enough for an assimilation of the data at ECMWF.

To conclude, we find the SCIAMACHY operational total ozone product has improved compared to the status in 2002 and 2003. Biases are of the order 0-4% for the tropics and mid-latitudes. Larger differences, up to 10%, are found at high latitudes or solar zenith angles. The noise on the product is low. Recently developed DOAS ozone column retrieval algorithms (including TOSOMI/TOGOMI) demonstrate the need for an upgrade of the SCIAMACHY operational processor. The KNMI TOSOMI product is available for the period January 2003 - present. It is a stable product which has shown an insensitivity towards level-1 product updates and shows a good agreement with the GOME data set processed with the TOGOMI algorithm. The monitoring with the ECMWF model has revealed problems with the ESA product during March and April 2004. There is a data gap in the near-real-time data and viewing geometry information is still missing in the meteo product.

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TEMIS project web site, http://www.temis.nl/.
