Near-real time delivery of GOME ozone profiles

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INTRODUCTION

In the framework of the ESA-DUP project GOFAP [1] the delivery of GOME ozone products in near-real time (NRT) to users has been accomplished. Since 1998 NRT ozone columns [2] are available through the KNMI website and since the beginning of 2000 they are accompanied by NRT stratospheric ozone profiles. Numerical weather prediction is expected to benefit from assimilation of stratospheric ozone profiles, if they are retrieved within 3 to 6 hours after observation. This requires a fast retrieval algorithm and a near-real time availability of the spectra. In this paper it is demonstrated that operational near-real time ozone profile retrieval for the use in weather forecast models is feasible.

The NRT ozone products of GOFAP are retrieved from specific segments of the full GOME spectrum contained in the EGOI files. These files are originally meant for instrument monitoring, but soon their suitability for NRT delivery of GOME products was recognised. Since the EGOI files contain raw data, a level 0-1 processor has been developed, partly based on the operational GDP processor.

For ozone profile retrieval the UV part (270-340 nm) of the GOME spectrum is used. The spectrum is measured with an integration time of 1.5 seconds, except for the spectrum below 283 nm, which has an exposure time of 12 seconds. Since GOME only measures spectra on the day side of each orbit, this implies that the processing time for one profile should not take longer than 24 seconds on average to keep up with the observations. A horizontal resolution of about 250 km suffices for weather forecasts (based on scales of nominal weather systems). The accuracy of the ozone profiles in the stratosphere should be better than the climatology presently used in the forecast models. Furthermore, a correct estimate of the accuracy is essential. There are no such requirements on the accuracy of the tropospheric part of the profile. To achieve a high accuracy in the stratosphere, several steps in the level 0-1 had to be improved, as shown by detailed validation studies on the quality of this level 1 data.

This paper will provide an overview of the accomplishments of the project, while details of the work will be given in dedicated papers.

LEVEL 0-1 PROCESSING

For each observation of GOME a selected part, the Extracted GOME Instrument header data (EGOI), is directly transmitted from the ground stations to ESRIN for instrument monitoring. The EGOI data consist of housekeeping information and 9 spectral windows of raw observation data (level 0). Since October 1999, the EGOI windows have been redefined to allow the retrieval of stratospheric ozone profiles in addition to the NRT column retrieval. The redefined spectral windows consist of 5 small windows of 2-10 nm width between 270 nm and 315 nm, 1 window around 330 nm of about 14 nm width, which is used for the ozone column retrieval, 2 windows around 352 nm and 373 nm of 1 nm width to aid in the derivation of the polarisation correction and the albedo, and a window around 770 nm, containing the O_2 A-band, used for cloud retrieval. An example of the calibrated EGOI data (level 1) in these spectral windows is shown in Fig 1.



Fig. 1. The calibrated EGOI data in 9 spectral windows. For each window the main purpose is stated. The reflectivity in window 2 is quite noisy due to the low radiance level and a short integration time in this window.

The ozone profiles are retrieved using the measured reflectances (proportional to the ratio of Earth radiance and solar irradiance) as a function of wavelength. The radiance calibration used is similar to the calibration performed in the offline GOME data processor ([3], [4]). However, some calibration steps in the off-line processor use the complete spectral information, and hence have to be adapted in the calibration of the confined EGOI data. For these calibration steps, stray-light correction and polarisation correction, a different approach is used. Also for the wavelength calibration, correction of the Peltier cooler interference, radiometric calibration and degradation correction a different approach is chosen. Details of these calibration steps can be found in [5].

NEAR-REAL TIME OZONE PROFILES

An existing off-line profile retrieval algorithm at KNMI [6] has been adapted to produce reliable stratospheric ozone profiles within the strict time constraint and with a spatial resolution sufficient for numerical weather predictions. For the retrieval the optimal estimation method [7] is used, utilising an iterative process to account for the non-linearity. For each iteration step the forward model is linearised by a weighting function. The weighting function is the derivative of the radiances to the ozone concentration at a number of altitudes. For the forward calculation the radiative transfer model MODTRAN 3.7 [8] is used. For each iteration, an optimal estimate profile is calculated from the profile of the former iteration step, the *a priori* information and the measured radiances. The *a priori* ozone profile is taken from the climatology of *Fortuin and Kelder* [9].

Since the off-line retrieval is not fast enough for the requirements, changes had to be made. The radiative transfer model is the most time-consuming part of the retrieval software. To minimise the calculation time spend on the radiative transfer model, the model has been optimised for speed and the number of required iterations has been reduced.

The reduction of the number of required iterations has been made possible by a better linearisation of the forward model by using the logarithm of the reflectivity (proportional to the ratio of earth-shine radiance and solar irradiance). A further reduction of calculation time is accomplished by using the weighting function of the previous step in some of the iteration steps.

The largest gain in calculation time is made by using a two-stream approximation for multiple scattering (hybrid delta-Eddington approximation [10]) instead of the more time-consuming DISORT multiple scattering calculation. This gives a negligible difference in the calculated radiances below 300 nm, but can differ up to 20 % for longer wavelengths. The consequence for retrieved ozone concentrations at lower altitudes (below 12 km) is that they deviate from the retrieved values using DISORT; on average 12 %. Minor differences (less than a few %) occur for the stratospheric values above 12 km, which are retrieved from the shortest wavelengths. For the purpose of weather forecasting only accurate values in the stratosphere are relevant. With these changes the processing of an ozone profile currently takes about 38 seconds. In the near-future a newly developed radiative transfer model of *van Oss and Spurr* [11] will be implemented. To be able to model reliable radiances above 300 nm, a fast and largely analytic radiative transfer model has been developed based on the LIDORT scheme of Spurr: LIDORT4A. This model produces radiances and weighting functions simultaneously using the discrete-ordinates method in the "4-stream" approximation.

Every 12 seconds GOME makes an observation in the UV spectrum suitable for profile retrieval. This observation has a ground pixel size of 960 by 100 km, resulting in global coverage in a period of 3 days. Each day GOME is producing more than 3000 observations, which are processed to ozone profiles. Since April 2000 the processing of NRT stratospheric ozone profiles is operational. The results can be found on URL *http://www.knmi.nl/gome_fd/*. More than 95 % of the profiles is available within 4 hours after the observation. Both resolution and time delay are within the requirements for operational use in weather forecast models.

Fig. 2 shows an example of the ozone distribution along an orbit of GOME on September 27, 2000 retrieved with the near-real time processor. The location of the orbit is around 130° W at about 19 hour GMT.

For numerical weather prediction the global 3D ozone distribution in the atmosphere can be estimated using data assimilation techniques. The first results of the data assimilation of the NRT ozone profiles are described in [12].



Fig. 2. Cross-cut of the calculated ozone distribution for an orbit of GOME at September 27, 2000. At 65 degrees South the border of the Antarctic ozone hole is clearly visible.

VALIDATION

A preliminary validation of the NRT ozone profiles is performed using satellite and situ measurements at the locations De Bilt (52.0 N, 5.1 E) and Paramaribo (5.8 N, 55.2 W). For the months November and December 1999 daily total ozone column measurements (if available) from the satellite instrument TOMS above the ground stations De Bilt and Paramaribo are compared to local measurements with a Brewer instrument. In addition, the integrated stratospheric ozone profiles (ISOP) of GOME above 120 mb are included in the ozone column comparisons. In Figure 3 this comparison is shown for the ground station at Paramaribo. To correct for the missing tropospheric part below 120 mb a fixed tropospheric ozone column of 30 DU has been added to the ISOP. The bottom panel of Fig. 3 shows the relative deviation with the Brewer measurements from Paramaribo. The average deviation from the Brewer measurement is 3.2 % for the ISOP values. The standard deviation on the differences with the Brewer values is 1.1 % (less than 3 DU).

The same comparison can not be made for De Bilt since the tropopause level is not always above 120 mb as is the case for the tropics and no simple correction can be given for the ozone column beneath 120 mb.



Fig. 3 Intercomparison for Paramaribo in 1999 between total ozone measurements from EP-TOMS (black plusses), the ISOP of GOME plus a fixed tropospheric column (red diamonds) and a Brewer (green stars).

In addition, the retrieved NRT ozone profiles from GOME are compared to ozone sonde measurements. Since ozone sondes are unreliable above 30 km (10 mb), such a validation is limited to the altitude range below 30 km. In Fig. 4 examples are given of ozone sonde measurements and collocated retrieved GOME NRT profiles at Paramaribo for November and December of 1999. In Fig. 5 this comparison is shown for collocated GOME NRT profiles at De Bilt in the same period. The retrieved ozone profiles in Paramaribo follows the sonde profile very well. At De Bilt deviations are larger, since the GOME profile can not resolve the high resolution features in the ozone profile. Note, that the GOME profile represents an average value for a ground pixel of 960 by 100 km, measured with a different temporal sampling compared to the ozone sounding. However, the deviations of the stratospheric values between GOME and the sonde are usual within the retrieval error (indicated with a horizontal bar in the Figures). For the profile above 10 mb comparisons with measurements from limb satellite instruments and lidar are planned.



Fig. 4 Collocated and coincidental ozone profiles measured by GOME and a sonde at Paramaribo. The *a priori* ozone profile is indicated with green diamonds.



Fig. 5 Collocated and coincidental ozone profiles measured by GOME and a sonde at De Bilt. The *a priori* ozone profile is indicated with green diamonds.

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