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for the PURPOSE of
OZONE PROFILE RETRIEVAL

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1. Introduction

The satellite instrument GOME [Burrows *et al.*, 1999], on board of the ERS-2 mission of ESA, is measuring backscattered sunlight from the atmosphere in the range from 240 to 790 nm. This spectrum is used for deriving globally, height-resolved information of the ozone distribution in the atmosphere [Chance *et al.*, 1997]. Contrary to total ozone column retrieval, the retrieval algorithm for ozone profiles requires absolutely calibrated reflectivity spectra. However, the in-flight calibration of the GOME reflectivity spectra needs to be corrected before the spectra can be used for profile retrieval. A method for this calibration correction of the GOME level 1 data is described in this report. The retrieved profiles from the recalibrated reflectivity spectra of GOME differ in the stratosphere up to 50 % from retrieved profiles without the correction. With the calibration correction improved ozone profiles are retrieved for the altitude range up to 50 km.

Several results from ozone profile retrieval from GOME data have been presented in the past [Munro *et al.*, 1998, Hoogen *et al.*, 1999, van der A *et al.*, 1998]. Munro *et al.* presented results of retrieved ozone profiles below 30 km. Hoogen *et al.* excluded the spectrum below 290 nm from their retrieval and corrected the spectrum above 290 nm with empirically derived Chebyshev polynomials. Their retrieved ozone values above the ozone maximum, however, show systematic deviations compared to ozone sondes. Comparison of our initial retrieved ozone profiles with ground measurements (from sondes of the NILU data base and lidar measurements) and ozone measurements from the satellite instrument HALOE revealed a strong systematic deviation above 25 km between GOME measurements and other ozone measurements. Ozone profiles from GOME retrieved for the upper stratosphere are not yet published in literature due to radiometric problems of the measured spectrum below 290 nm. In this report these problems are identified, and subsequently corrected for, in order to be able to present accurate ozone profiles for both troposphere and stratosphere.

2. Radiometric calibration GOME

A few case studies have been performed to compare the reflectivities measured by GOME with model results. The calibrated GOME reflectivities are given by the GOME Data Processor version 2.0 [Balzer *et al.*, 1996] including an instrument degradation and BSDF correction [Aben *et al.*, 1999, Hegels and Slijkhuis, 1999]. It is assumed that the degradation of the instrument affects the measured solar spectrum and Earthshine spectrum in a similar way. Since the reflectivities are calculated from the ratio of these spectra, they are unaffected by the degradation correction. The modelled reflectivities are calculated by the radiative transfer model MODTRAN 3.7 [Berk *et al.*, 1989, Anderson *et al.*, 1995], where a collocated and co-temporal ozone measurement from a ground station serves as input. The Ring effect [Grainger and Ring, 1962, Joiner *et al.*, 1995] on the GOME reflectivity spectrum is accounted for by applying a pre-calculated "Ring spectrum" [Chance and Spurr, 1997].

These case studies show measured reflectivities in the UV, which are typically about 30 % higher than expected from the model results. A few typical examples of a comparison between model and measurement are shown in Figure 1 for a GOME observation at the position of a ground station, where a ground measurement has been performed on the same day. Although the theoretical spectrum is corrected for the Ring effect, some spectral features are still visible at 280 nm and 285.3 nm at the position of the Mg II Fraunhofer lines of the solar spectrum. This indicates an offset in the Earthshine spectrum resulting in higher values of the measured reflectivity at the solar lines, where the intensity is the lowest.

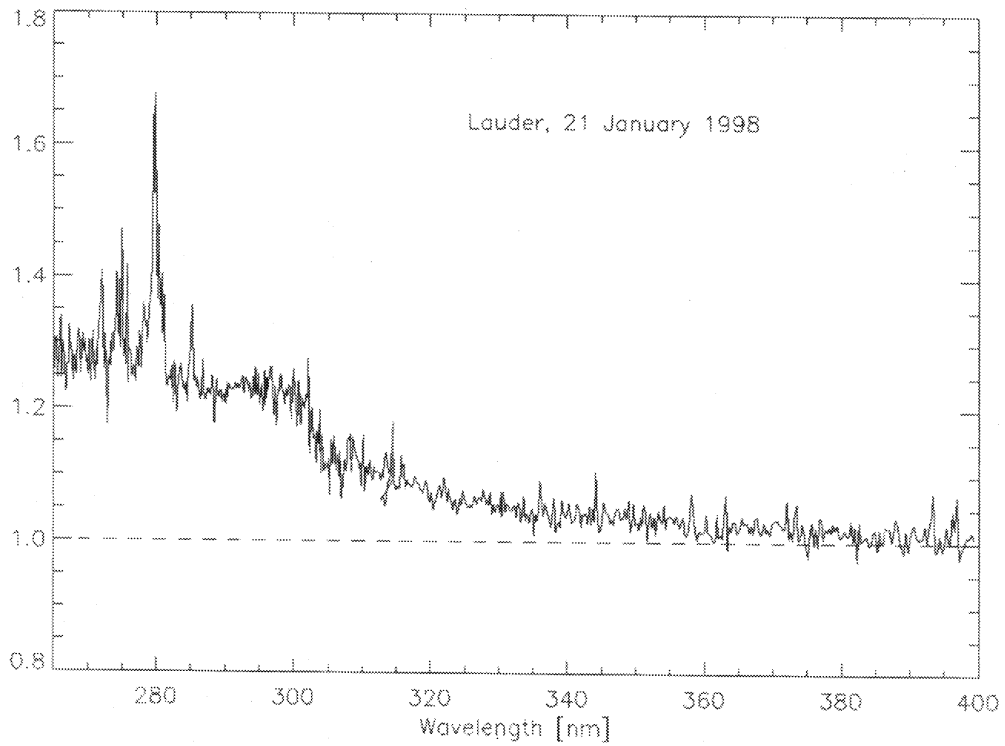


Figure 1a Ratio of the measured reflectivity spectrum and the modelled reflectivity spectrum at 21 January 1998 above Lauder, New Zealand. The modelled spectrum is based on the coincidental and collocated ozone profile of a combined lidar and ozone sonde measurement at Lauder.

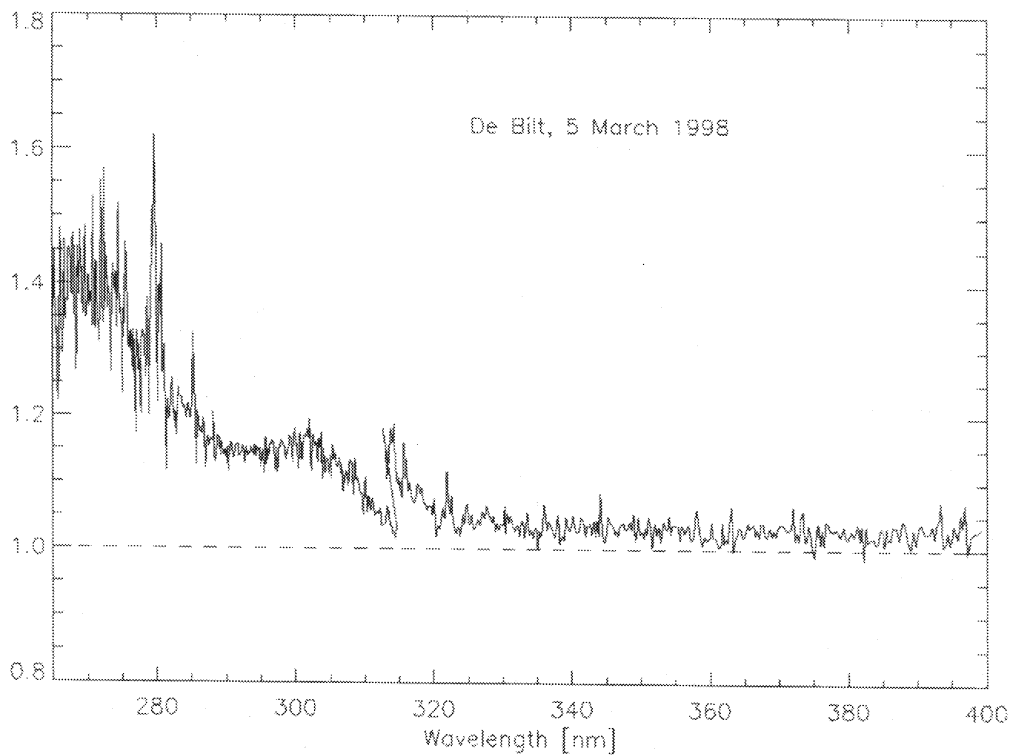


Figure 1b Ratio of the measured reflectivity spectrum and the modelled reflectivity spectrum at 5 March 1998 above De Bilt, The Netherlands. The modelled spectrum is based on the coincidental and collocated ozone profile of an ozone sonde measurement at De Bilt.

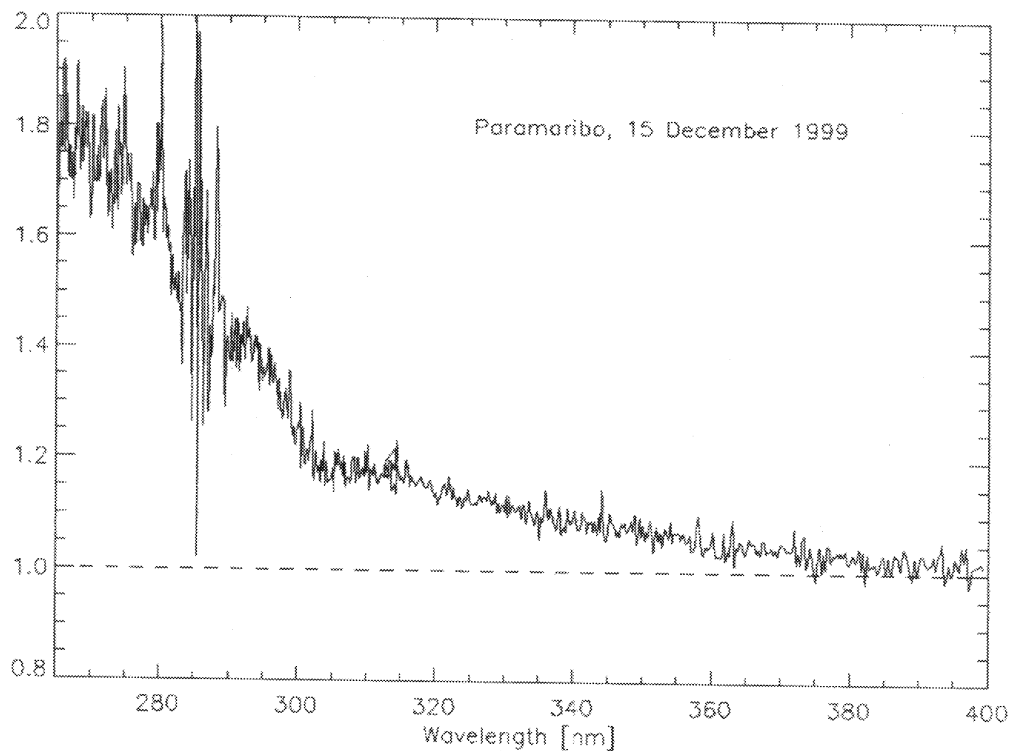


Figure 1c Ratio of the measured reflectivity spectrum and the modelled reflectivity spectrum at 15 December 1999 above Paramaribo, Suriname. The modelled spectrum is based on the coincidental and collocated ozone profile of an ozone sonde measurement at Paramaribo.

Comparison between measured SBUV/2 reflectivities and GOME reflectivities observing the same ozone mass also show higher values (5-30 %) for GOME in the UV below 300 nm [L.E. Flynn and Y. Pachepsky, private communication, 2000]. The differences are too large to be explained by differences in geometry. Also, for similar solar zenith angles and solar azimuth angles the average radiance in the UV measured by SBUV/2 is much lower than the average radiance measured by GOME.

The radiance at top-of-atmosphere below 300 nm is largely due to single scattering and has only a very small contribution from the ground. Therefore we do not expect large errors in the modelled radiances. Still, to be sure, the results from the radiative transfer model MODTRAN 3.7 used in this study have been compared to the radiative transfer models DAK [de Haan *et al.*, 1987], MODTRAN version 4.0 and LIDORT [Spurr *et al.*, 2001] for several geometrical situations. As expected, no significant differences in the model results were found for the wavelength range 260 to 300 nm.

The known errors in the radiative transfer calculation due to aerosol contributions, temperature profile deviations, Ring effect and polarisation in the atmosphere are too small (less than a few percent) to explain the differences with the GOME measurements. No discontinuity is visible in the average spectrum at 283 nm, where the boundary is between channel 1a and 1b, each read-out with a different exposure time. Therefore, possible effects of non-linearity or an electronic offset in the instrument can not explain the behaviour of the calibration differences as function of intensity. An error in the polarisation correction of the instrument would also be too small to explain the differences below 300 nm.

The degradation of the solar spectrum is regularly checked and calibrated with SOLSTICE (see e.g. Peeters and Simon, 1996). Since this degradation is used to correct both solar irradiances and Earth radiances in the GOME level 1 data extractor, we assume that the measured Earth radiances degrade differently and, therefore, are not correctly calibrated. An incorrect calibration is also suggested by an earlier study of Hilsenrath *et al.* (1996), which shows a mismatch in radiance levels below 340 nm of at least 10 percent. The moon measurements of GOME have been analysed in order to assess the degradation of the measured Earth radiances [Snel, 1999, Haman and Burrows, 1999], but these

studies were hampered by low signal-to-noise ratios and did not result in any conclusions concerning Earth radiance degradation. Therefore a new method is introduced to make an assessment of the radiance calibration below 340 nm, which is relevant for ozone profile retrieval.

3. Recalibration of the Earthshine radiances

The mismatch in the GOME calibration as identified in the previous section can be corrected in three steps: a correction of a wavelength independent offset, a wavelength dependent radiometric correction and a time dependent correction for the degradation of the instrument.

To correct the offset in each spectrum the solar Fraunhofer line at 280 nm is used. The ozone cross-section between 278 and 282 nm does not change very much, so that we can assume that the reflectivity at 280 nm, R_{280} , is the average of the reflectivities at 278 nm and 282 nm, respectively R_{278} and R_{282} :

$$R_{280} = \frac{1}{2} (R_{278} + R_{282}) \quad [1]$$

The reflectivity R_λ at a wavelength λ is defined as $R_\lambda = \pi I_\lambda / \mu F_\lambda$, where I_λ is the measured Earth radiance, μ is the cosine of the solar zenith angle and F_λ is the measured solar irradiance at wavelength λ . When a constant offset C is present in the measured Earth radiance, the correct reflectivity can be calculated from the measured reflectivity R'_λ , according $R_\lambda = R'_\lambda - \pi C / \mu F_\lambda$. Any offset in the measured solar spectrum can be neglected because the measured signal of the solar spectrum is much higher. Using relation [1] the offset can be derived for each spectrum according to

$$C = \frac{\mu}{\pi} \frac{R'_{278} + R'_{282} - 2R'_{280}}{F_{278}^{-1} + F_{282}^{-1} - 2F_{280}^{-1}} \quad [2]$$

Furthermore, the radiometric response function of the instrument has been incorporated in the calculation. The calculated offset has a weak correlation (about 0.3) with the total radiance of the spectrum in channel 1, which suggests part of the offset being related to uncorrected straylight. A stronger correlation of about 0.75 has been found between the offset and the conduct signals of the Peltier cooler. The interference of the Peltier cooler conduct signals on the detector signal is a known problem of the GOME reflectivity spectrum, for which a correction is included in the standard radiometric calibration of the GOME data processor. However, the remaining correlation shows that the above described offset correction is necessary to deal with the remaining effects of the interference signal.

The average offset, which is probably related to an imperfect straylight correction, is on average about $7.2 \cdot 10^8$ photons \cdot s $^{-1}$ sr $^{-1}$ cm $^{-2}$ nm $^{-1}$ and the variation in the offset due to interference of the Peltier cooler is of the same order of magnitude. The effect of the offset correction on the Earth radiances above 290 nm or the solar spectrum can be neglected.

To identify the remaining mismatch in the calibration of the Earthshine radiances, we have compared about 3500 representative measured spectra of GOME in the period 1995 to 2001 with model results. The spectra are taken from randomly chosen orbits covering all latitudes on the days of 23/07/95, 06/04/96, 04/08/96, 06/04/97, 03/08/97, 06/04/98, 04/08/98, 06/04/99, 04/08/99, 16/12/99, 17/12/99, 24/03/00, 27/06/00, 13/08/00, and 02/01/01. Most of the longitudes are covered, but none of the orbits is located at the South Atlantic Anomaly, where the spectra in the UV are seriously deteriorated by the impact of cosmic high-energy particles on the detector. For each measurement the effective ground albedo has been obtained from the measured reflectivity at 400 nm, where the trace gas absorption is minimal. For each measurement we have performed MODTRAN simulations with the *Fortuin and Kelder* (1998) ozone climatology and the calculated albedo as input. This climatology consists of zonal mean, monthly ozone values based on a 12-year observation period of ozone sonde stations and the SBUV and TOMS satellite instruments. The ratio of each measured and modelled

spectra is calculated. The mean of the ratio f_λ at each wavelength of the spectra (from an ozone profile ρ with index i) within an orbit is used to average out differences due to ozone variations $\Delta\rho$ from the climatology $\bar{\rho}$. For each wavelength, the ratios are averaged over i :

$$f_\lambda = \left(\frac{I(\rho_i)}{I_{\text{model}}(\bar{\rho}_i)} \right)_\lambda = \left(\frac{I(\bar{\rho}_i) + \Delta I(\Delta\rho_i)}{I_{\text{model}}(\bar{\rho}_i)} \right)_\lambda \approx \left(\frac{I(\bar{\rho}_i)}{I_{\text{model}}(\bar{\rho}_i)} \right)_\lambda \quad [3]$$

To remove any residual features of the Ring effect, the spectrum is smoothed with a running average of 2 nm width. Deviations up to 40 % were found between model results and GOME measurements. No significant solar zenith angle or latitude dependence could be identified, so we take the ratio f_λ to be valid for each spectrum in an orbit.

Apart from the deviation of the radiometric calibration, we observed that the deviation starts to grow from the end of the year 1998, notably at the shortest wavelengths (< 300 nm). In the calibration of the GOME data processor, a degradation correction is applied, but there it is assumed that the solar spectrum and Earthshine spectrum degrade in the same way. However, our results show that the ratio of these spectra, the reflectivity, starts to increase from 1998, which indicates a faster degradation of the solar measurements. The reflectivity degradation for the shortest wavelengths has been parameterised for each wavelength with a polynomial as function of time. The identified degradation correction as function of wavelength is shown in Figure 2a for a few days in the period 1998 to 2001. The degradation correction for a few wavelengths as function of time is shown in Figure 2b.

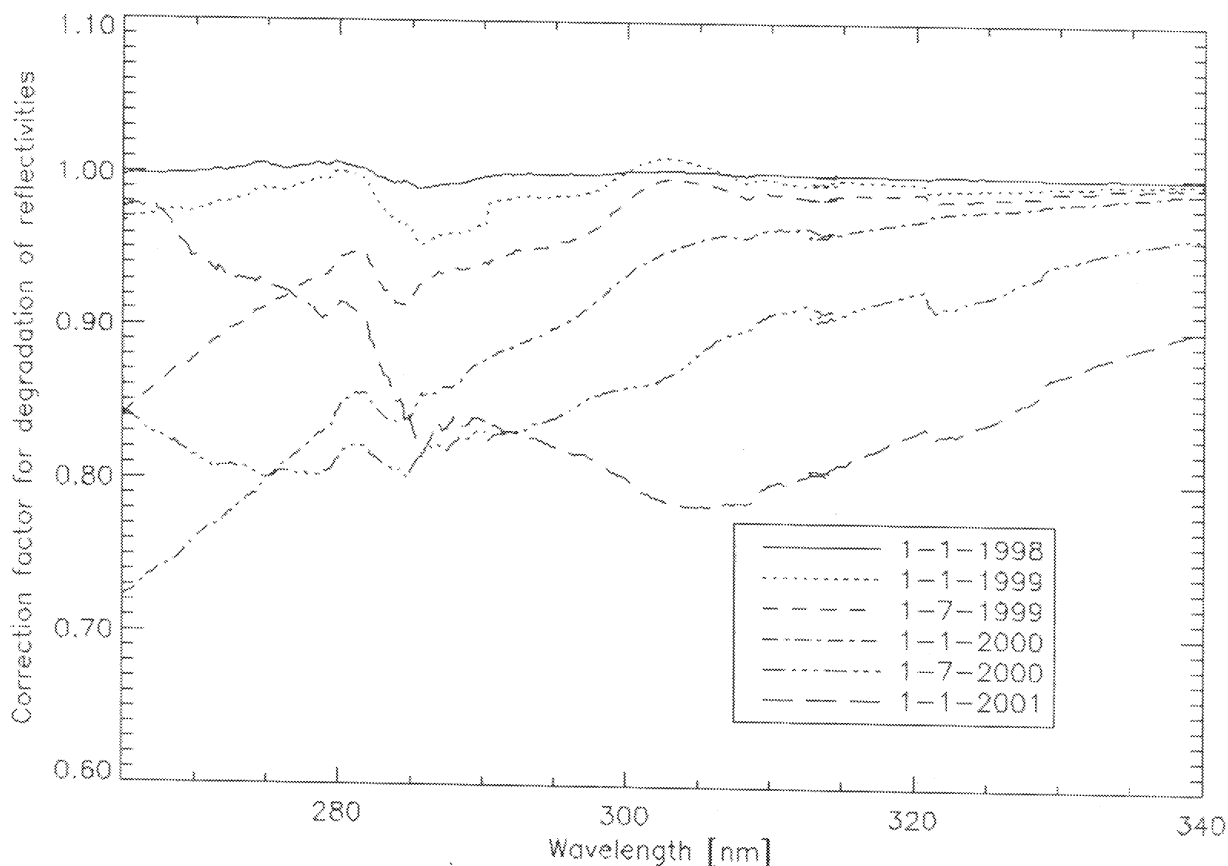


Figure 2a The degradation factor indicated as the reflectivity spectrum compared to the average reflectivity spectrum of the years 1995 up to 1997. Significant degradation started after 1998.

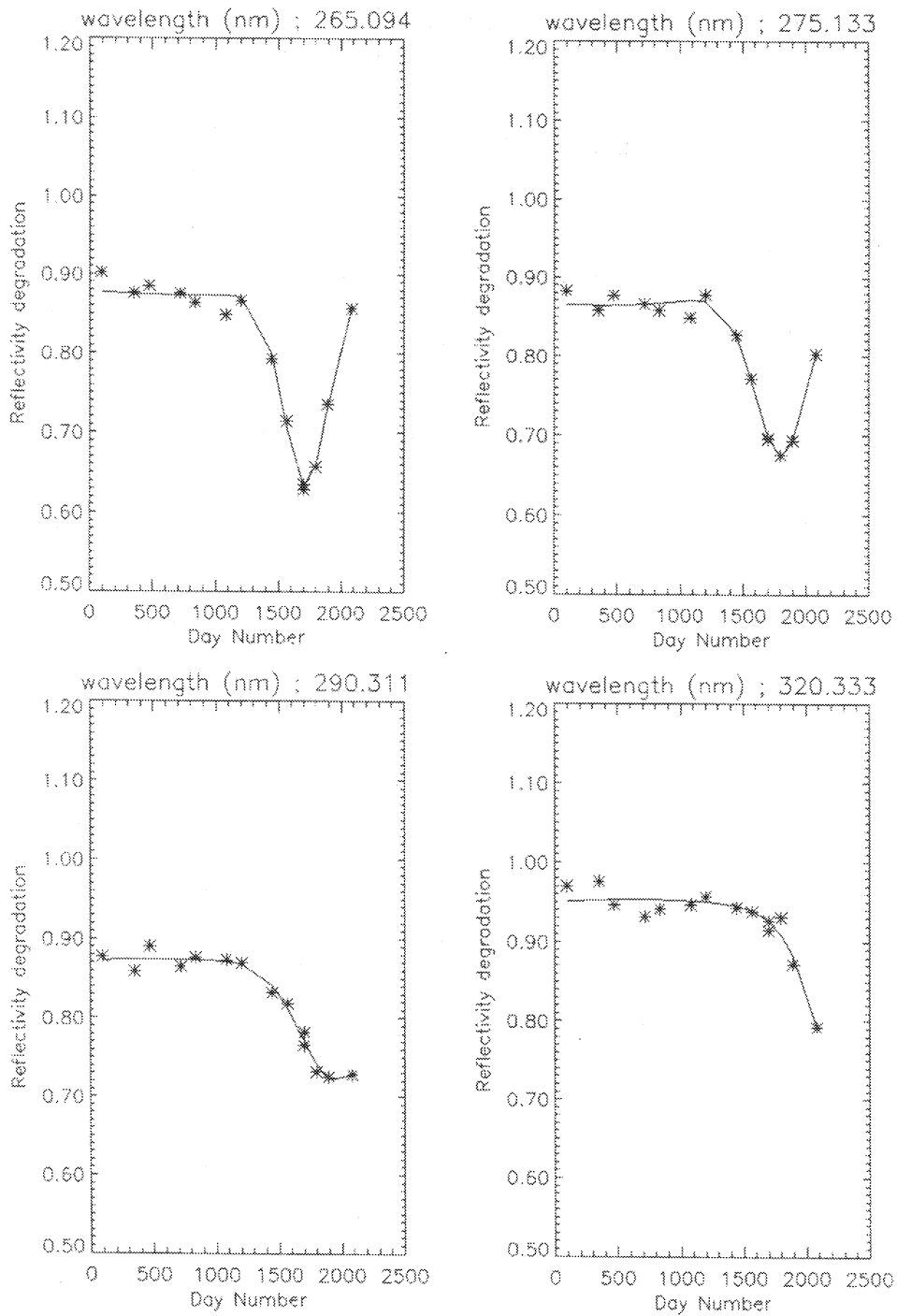


Figure 2b The degradation correction factor as function of time for a few wavelengths in channel 1 and 2 of GOME. The time is given in days after the launch of GOME on the ERS-2 platform; e.g. day number 2000 is October 11, 2000.

Based on these results a parameterised correction function has been developed for the radiometric calibration including the degradation. Figure 3 shows the radiometric correction as function of wavelength when no degradation is present, as was the situation before 1998. The deviation in the UV is too large to be explained by biases in the ozone climatology. The calculated standard deviation shown in Figure 3 tells us that natural statistical fluctuations in ozone can not explain the differences between model and measurement. A possible explanation for the deviations at the early orbits can be the different response from a variable scan mirror angle as used in in-flight measurements and the response from a fixed scan mirror angle as used at the ground calibration of GOME. This would also explain the different radiometric calibration deviation found in a similar comparison for measurements of the small swath observations and of the forward pixels of GOME, which are measured at different scan mirror positions (see Figure 4).

Clearly visible in Figure 3 is the difference of about 1 to 2 % in calibration of the instrument in the channel overlap (between channel 1 and 2) region around 313 nm. This discrepancy is also fixed with the radiometric correction factor. The fine structure of the calibration correction is probably caused by a residual of the Ring effect.

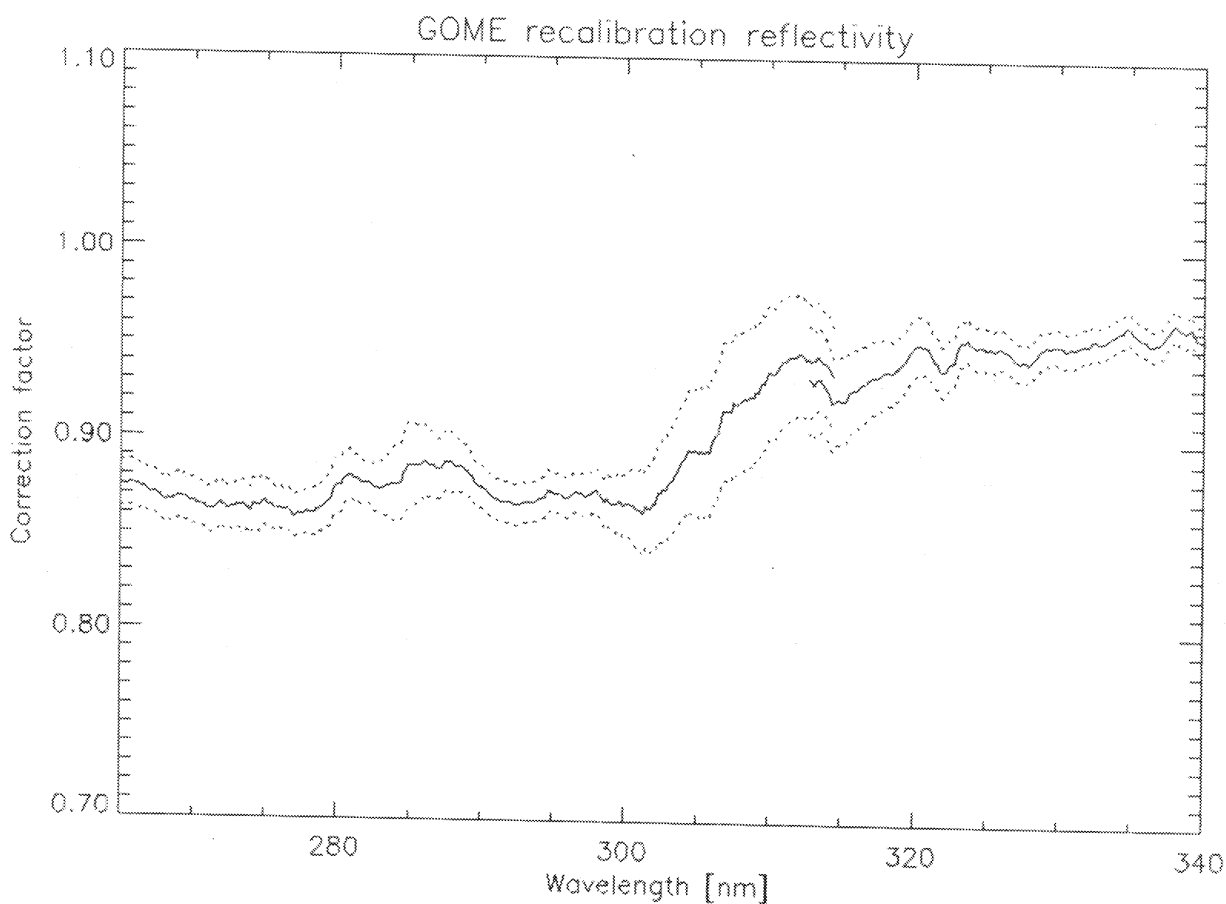


Figure 3 Correction for the radiometric calibration of the GOME reflectivity spectrum based on the comparison between model and measurement for a series of representative spectra in the period June 1995 till April 1998. The dotted lines indicate the standard deviation on the correction factor.

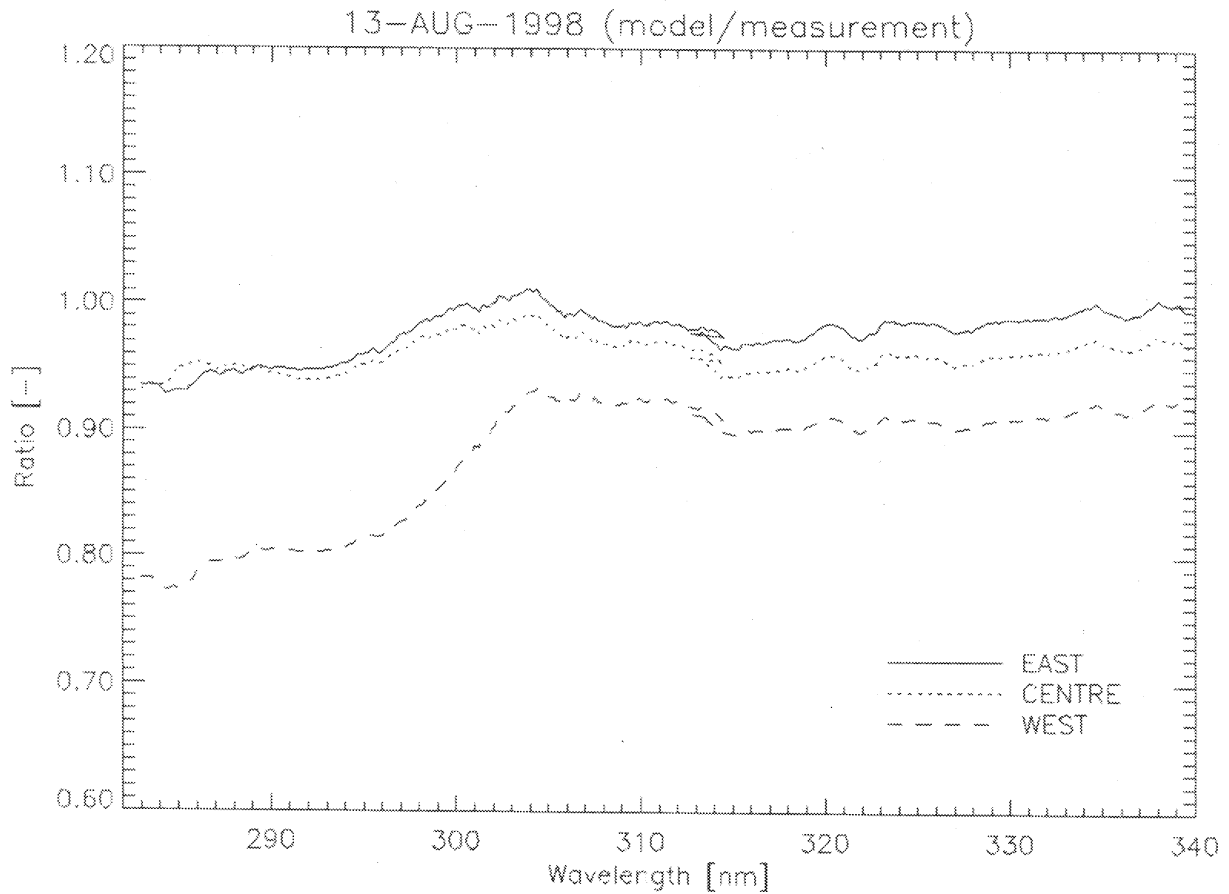


Figure 4 Correction for the radiometric calibration of the GOME reflectivity spectrum for the forward pixels, as derived for the instrument on August 13, 1998.

Figure 5 demonstrates the effect of the offset, calibration and degradation correction on the retrieved ozone profile. An ozone profile has been retrieved, with and without correction of the radiance spectrum, from a GOME observation above Lauder at January 21, 1998. At the same day an ozone sonde and lidar measurement was performed. Below 25 km there were no significant differences between both retrieved profiles of GOME. Above 25 km, however the differences can be as high as 50 percent, resulting in a better resemblance with the collocated ground measurement.

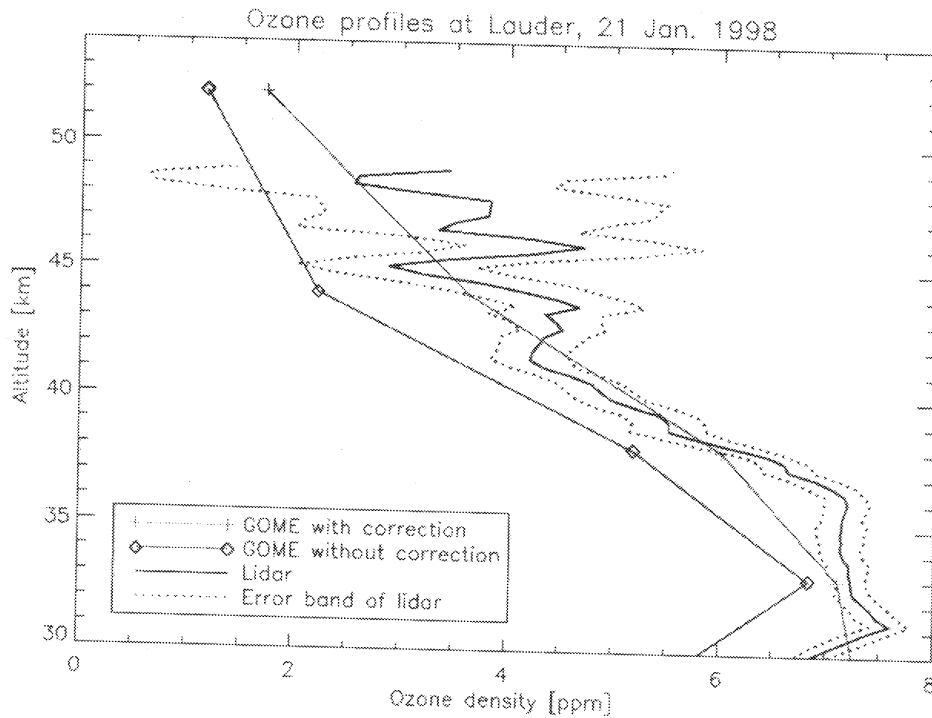


Figure 5 Comparison of a retrieved ozone profile with and without correction of the reflectivity spectrum. The collocated and coincidental ground observation from a lidar is also shown, including the error margins of the lidar measurement.

4. Conclusions

Because the ozone profile retrieval is sensitive to absolutely calibrated reflectivities, the accuracy of the retrieved profiles depends strongly on the quality of this reflectivity spectrum. Validation of many reflectivity spectra during the operation of GOME with model results and SBUV/2 spectra showed several systematic inadequacies of the spectra. Identified were interference of the Peltier cooler, degradation of the reflectivities and a mismatch in the radiometric calibration of the Earth radiances. Correction methods have been developed and applied in the retrieval procedure to account for these systematic errors. The correction involves three sequential steps :

1. Correction of an offset at the Earth radiance spectrum in order to remove residual effects of the interference of the Peltier cooler signals.
2. Correction of the radiometric calibration of the instrument.
3. Correction of the different degradation of Earth radiances as compared to the solar irradiance spectrum.

The radiometric correction algorithm we derived for GOME UV spectra can be downloaded from the URL <http://www.knmi.nl/~avander/GOME/calibration.html>.

The retrieved profiles from the recalibrated reflectivity spectra of GOME differ in the stratosphere up to 50 % from retrieved profiles without the corrections. Comparisons to ozone sondes, lidar measurements and HALOE measurements show that the newly retrieved ozone profiles based on recalibrated GOME data agree significantly better with the sonde/lidar measurements in the stratosphere.

Although the reflectivities can be corrected, the signal-to-noise ratios of the measurements are irreversibly reduced due to the degradation in the course of the mission. This reduction can amount to

50 % in the spectra below 300 nm in the year 2000. Another conclusion is that trend studies in retrieved profiles from GOME are seriously hampered by the difficult distinction between degradation and trend effects in the measured spectra. It has to be noted that the method described in this section using model studies to correct degradation does not solve this side effect.

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