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Advances in Space Research 34 (2004) 749–753
ADVANCES IN SPACE RESEARCH (a COSPAR publication)
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Application of a modified DOAS method for total ozone retrieval from GOME data at high polar latitudes

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Received 1 December 2002; received in revised form 25 April 2003; accepted 23 May 2003

Abstract

Since 1995, the Global Ozone Monitoring Experiment (GOME) on board the second European Remote Sensing satellite provides information about spatial distribution and temporal variation of total ozone. Current operational data products are generated using the Differential Optical Absorption Spectroscopy (DOAS) technique. Various validation exercises indicate shortcomings in the current retrieval using the standard DOAS approach. Especially under ozone hole conditions at high polar latitudes GOME tends to overestimate total ozone as compared to ground-based measurements. In this study, we introduce a modified DOAS method for ozone retrieval from GOME which fits directly the vertical columns rather than slant columns. We present preliminary results which demonstrate the advantage of the new approach. It will be shown that not only the differences to ground-based data are reduced but also the fit residuals are improved in comparison with the operational retrieval.

Keywords: GOME satellite data; Total ozone retrieval; High polar latitudes; Differential optical absorption spectroscopy

1. Introduction

The stratospheric ozone layer screens the Earth's environment from solar ultraviolet radiation which has harmful effects on processes in the biosphere. Since Farman et al. (1985) detected dramatic changes in the ozone concentration during Antarctic spring, the need for accurate global measurements arose. For this purpose satellite instruments have been designed to achieve a global view of the atmospheric system.

The Global Ozone Monitoring Experiment (GOME) has been launched in 1995 on board the second European Remote Sensing satellite (ERS-2) (Burrows et al., 1999b). The instrument measures the earthshine radiance and solar irradiance in nadir viewing geometry from 240 to 790 nm with moderate spectral resolution (0.2–0.4 nm). After seven years of operation it provides a unique long-term dataset of global ozone measurements which are operationally derived using the Differential Optical Absorption Spectroscopy (DOAS) method (Platt and Perner, 1980). The so called slant column density is first derived from a spectral fit to the logarithm of the sun-normalized radiance and then converted into vertical column density using an airmass factor (AMF) computed with radiative transfer models (RTM). Comparison between GOME Data Processor (GDP) V2.70 (Spurr, 1996) and ground-based data show a marked seasonal variation, which is reduced but still present in the current GDP V3.00 products (Lambert et al., 2002). The most likely explanation is the difficulty in deriving the AMF (Lambert et al., 1999; Bramstedt et al., 2003).

In this study, we present a modified DOAS algorithm, weighting function modified DOAS (WFM-DOAS, Buchwitz et al. (2000)), that eliminates the need for an AMF conversion. Investigations concerning the influence of ozone and temperature profiles are shown using simulated data. Finally, the new method is applied to GOME data from high polar latitudes under ozone hole conditions, demonstrating the potential improvement to be expected from WFM-DOAS.

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doi:10.1016/j.asr.2003.05.051

2. Weighting function DOAS approach

2.1. Theory

The weighting function modified DOAS algorithm has been originally developed for trace gas retrieval in the near-infrared spectral range measured by Scanning Imaging Absorption Spectrometer on Atmospheric Chartography (SCIAMACHY) (Buchwitz et al., 2000). However, the algorithm is not limited to a particular wavelength range and molecular line absorbers. It is directly transferable to ozone retrieval in the ultraviolet (UV) spectral range requiring only minor modifications. The measured optical depth ($\ln I_i^{\mathrm{mea}}$) is approximated by a linearized radiative transfer model ($\ln I_i^{\mathrm{mod}}$) plus a low-order polynomial P_i (see Eq. (1)), the latter accounting for broadband contributions. The total column information is obtained from differential trace gas absorption structures as in standard DOAS. The equation can be written as follows:

$$\begin{aligned}\ln I_i^{\mathrm{mea}}(V^{\mathrm{t}},\vec{b}^{\mathrm{t}}) \approx \ln I_i^{\mathrm{mod}}(\bar{V},\bar{\vec{b}}) + \left.\frac{\partial \ln I_i^{\mathrm{mod}}}{\partial V}\right|_{\bar{V}} \\ \times (\hat{V}-\bar{V}) + \sum_{j=1}^{F} \left.\frac{\partial \ln I_i^{\mathrm{mod}}}{\partial b_j}\right|_{\bar{b}_j} \\ \times (\hat{b}_j - \bar{b}_j) + \mathrm{SCD}_{\mathrm{Ring}} \cdot \sigma_{i,\mathrm{Ring}} \\ + \mathrm{SCD}_{\mathrm{usamp}} \cdot \sigma_{i,\mathrm{usamp}} + P_i, \qquad (1)\end{aligned}$$

where I^{mea} is the measured intensity and I^{mod} the reference intensity, as provided by the RTM. Index t denotes the true atmospheric state. The entire right-hand side of the equation has to be adjusted to the measured intensity at all spectral points (index i) simultaneously. $\bar{V}$ is the reference ozone column matched to the reference intensity and $\hat{V}$ the retrieved vertical column (fit parameter). $\vec{b}$ contains all other contributing atmospheric parameters such as temperature, and interfering trace gases. In case of ozone retrieval in the UV, NO_2 and BrO are important. All reference parameters are denoted by overbars and all fit parameters are denoted by hats. Ring effect $\sigma_{i,\mathrm{Ring}}$ and undersampling spectrum $\sigma_{i,\mathrm{usamp}}$ are treated as effective absorbers similar to the standard DOAS approach. A slant column fit is performed for both.

The main difference between WFM-DOAS and standard DOAS is the use of wavelength dependent weighting functions (WF) instead of absorption cross sections and AMF. Weighting functions describe the relative radiance change due to a vertical profile change assuming an altitude independent scaling factor. The need for an AMF conversion is eliminated in the new algorithm as the vertical columns are fitted directly. By introducing additional terms in vector $\vec{b}$ the algorithm is able to compensate effects related to other unknown atmospheric parameters. The unknown fit parameters are derived using a linear least-squares minimization as in standard DOAS.

2.2. Algorithm description

Since calculations of weighting functions and reference intensity with a full RTM is computationally quite expensive, all quantities are provided in look-up-tables (LUT). In order to retrieve total ozone columns globally, a large set of reference spectra has to be built up which must include nearly all possible atmospheric states. The radiance spectra and weighting functions are computed as a function of total ozone (including profile shape), zonal band (tropics, mid latitude and polar), solar zenith angle (SZA), line-of-sight, surface albedo, and altitude for the spectral region from 325 to 335 nm which has been selected for the fit. The SCIATRAN code, an extension of the GOMETRAN++ radiative transfer model (Rozanov et al., 1997) was used to determine altitude resolved weighting functions quasi-analytically (Rozanov et al., 1998). The LUT then contains the height integrated weighting functions. Table 1 gives an overview on the selected parameters and their spacing. For the calculation GOME FM ozone cross-sections (Burrows et al., 1999a) are used. Ozone and temperature profiles are taken from the TOMS Version 7 climatology (Wellemeyer et al., 1997), which contains different profile shapes for three latitude belts (low, middle and high) as a function of total ozone column. The relative azimuth angle (RAZ) between illumination and observation is assumed to be accurately defined by the SZA and line-of-sight as the GOME data indicate a relatively small variation of the RAZ with a certain

Table 1
Parameter space of look-up-table

Atmosperic parameter	Minimum	Maximum	Δ	N
Total ozone (high latitudes)	125 DU	575 DU	50 DU	10
Total ozone (mid latitudes)	125 DU	575 DU	50 DU	10
Total ozone (low latitudes)	225 DU	475 DU	50 DU	6
Solar zenith angle	15°	92°	5° if $\leqslant$ 70°; 1° if > 70°	34
Line-of-sight	−34.5	−34.5	11.5	7
Surface albedo	0.02	0.98	~ 0.2	6
Ground altitude	0 km	12 km	2 km	7

combination of SZA and line-of-sight. Errors in vertical ozone columns of up to ±0.5% are expected when neglecting this variation as theoretical studies have shown. Only one aerosol scenario (maritime type) given by the Lowtran model has been selected for the LUT. Additional scenarios are necessary for the planned global ozone retrieval from GOME. An iterative scheme is used to find the reference scenario which most closely matches the real atmospheric state. Input data are the viewing geometry taken from GOME level 1 data, ground altitude, and the Lambertian equivalent reflectivity at 377 nm. The operational ozone product is used as first guess for the fit. The retrieved column is then compared to other available ozone columns in the LUT. If there is an ozone column which is closer to the retrieved one, the fit is repeated, while all other parameters are kept fixed.

In case of cloud contaminated GOME ground pixels, the part of the ozone column which is below the cloud top cannot be seen by the satellite. A ghost vertical column (GVC) has to be estimated from climatological ozone profiles and is added to the column retrieved from the spectral fit. The GVC is computed by integrating the ozone profile from the surface to cloud top pressure taken from the International Satellite Cloud Climatology Project (Rossow and Garder, 1993). Partial cloudiness can be taken into account by weighting the GVC with fractional cloud cover which is derived using the Initial Cloud Fitting Algorithm (ICFA, Kuze and Chance (1994); Burrows et al. (1999b)).

3. Theoretical studies

First studies concerning the application of weighting function DOAS have been performed using synthetic spectra. The influence of differences between real atmospheric ozone and temperature profiles and those profiles used for the calculation of the reference spectra has been investigated. Twelve radiance spectra were computed using different ozone and temperature profiles for high latitudes (January–December, 65°N) taken from 2D model calculations performed at the Max-Planck-Institute (MPI) in Mainz, Germany (C. Brühl, personal communication, 1992). The MPI 2D climatology is currently used to determine the AMF in GDP V2.70. The reference spectra used in the fitting procedure were calculated with only one ozone and temperature profile taken from the TOMS V7 climatology for high latitudes. All ozone profiles were scaled to 325 DU. SZA varied from 50° to 80° and albedo was 0.05. Large deviations between TOMS V7 and MPI profiles occur which may reach 20 K between 35 and 40 km. Fit results for all 12 synthetic spectra are shown in Fig. 1. If the temperature WF is not included in the fit, deviations of up to 12% between retrieved columns and correct columns are obtained. The temperature weighting function reduces those differences to below 5%. Largest errors occur in winter (January and December) when SZA was 80°. Fig. 2 shows a comparison between the temperature from MPI climatology at the altitude of maximum ozone concentration (21 km) and the temperature retrieved in the WFM-DOAS fit. The algorithm is able to reproduce the correct temperature with errors smaller than 2% if the SZA is below 70°. Additionally, a correlation to the differences in ozone column is found. Overestimation of ozone column belongs to underestimation of atmospheric temperature and vice versa, which is explained by positive correlations between temperature and ozone weighting functions.

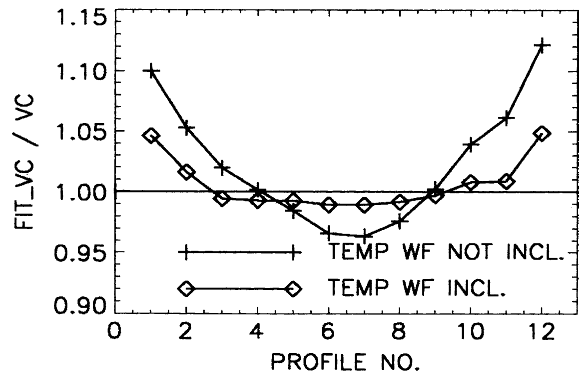

Fig. 1. Ratio of WFM-DOAS vertical column to correct vertical column with temperature weighting function included (diamonds) and without including temperature WF (crosses).

The new GDP version 3.0 also takes the temperature dependence into account by fitting two O_3 cross sections measured at different temperatures. Besides the ozone slant column, the absorption effective temperature is retrieved. Several studies have been performed by Van Roozendael et al. (2002) which indicate a significant reduction of the fit root-mean-squared error (RMS).

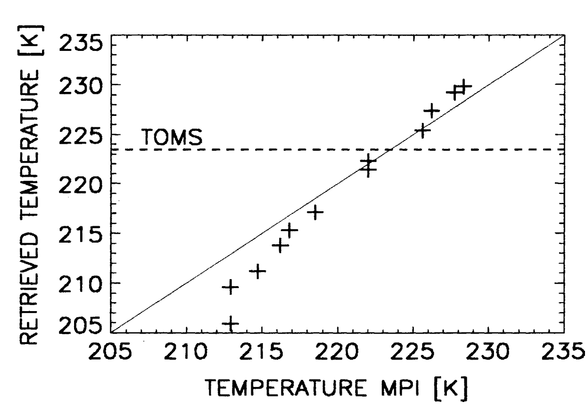

Fig. 2. Retrieved temperature against MPI climatology temperature at the altitude of maximum ozone concentration (21 km). Dashed line: temperature from reference profile (223.5 K).

4. Application to GOME data from high polar latitude

First investigations using GOME satellite data have been performed under ozone hole conditions at high southern polar latitude. We selected the period from September to December 1997 and two locations in Antarctica, Neumayer Station (70°S, 8°W) and Belgrano II Station (77°S, 34°W). The data were provided by the World Ozone and UV Radiation Data Centre (WOUDC) through their website (http://www.msc-smc.ec.gc.ca/woudc/woudc.html). The data from Neumayer are ozone columns derived from sonde ascents approximately every fifth day. At Belgrano II a Brewer spectrometer is installed, and daily means were computed. All measurements are checked for GOME overpasses the same day. The maximum distance between pixel center and station geolocation is 160 km. Twenty four collocations were found for Neumayer Station, and 73 were found for Belgrano II. Those data with less than 10 Brewer measurements per day have not been taken into account, as well as those days where sulfur dioxide column is extremely large. SO_2 and ozone are measured simultaneously with Brewer spectrometers. SZA varied between 80° in September and 45° in December.

Ratios between collocated satellite results and ground-based data were determined. The mean difference to sonde data is 12% for GDP V2.70 data products, 4% for GDP V3.00 data, and 1% for the WFM-DOAS retrieval. RMS is reduced from 16% (GDP V2.70) to 8% (GDP V3.00 and WFM-DOAS). The results are shown in Fig. 3. The large overestimation which occurs in GDP V2.70 data, when total ozone column is below 220 DU (day 4–16) is reduced by using WFM-DOAS, but also in the current V3.00 products (left panel). Such an improvement is obtained mostly due to the implementation of an effective ozone temperature fitting (GDP V3.00) and the use of temperature weighting functions (WFM-DOAS), respectively. GDP V3.00 and WFM-DOAS both use the TOMS V7 ozone climatology instead of the MPI 2D profiles which may be another reason for similar results.

Another promising result is the reduction of the fit residual of the WFM-DOAS retrieval by more than 55% compared to V2.70 and by 15% compared to V3.00 as presented in the right panel of Fig. 3. This may be due to the use of wavelength dependent weighting functions instead of a single AMF at one wavelength for the whole fitting window as done in standard DOAS (Burrows et al., 1999b). The single AMF approach is insufficient

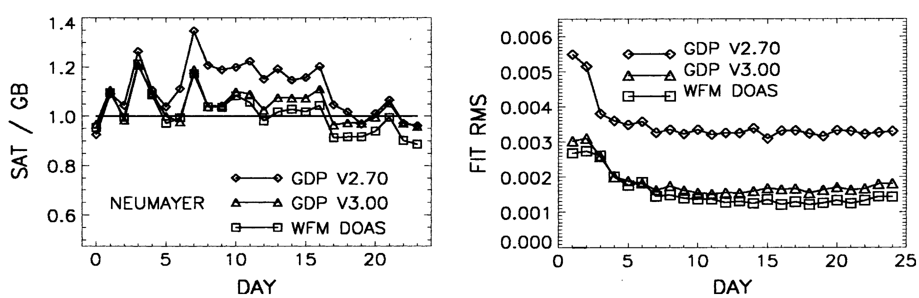

Fig. 3. Ratio of ozone column derived from satellite measurements to ozone column derived from sondes at Neumayer Station as function of time from September to December (left), and root-mean-squared error of the spectral fit for both retrieval algorithms standard DOAS and WFM-DOAS (right). Diamonds denote GDP V2.70 data, triangles denote GDP V3.00 data, and squares denote the new WFM-DOAS values.

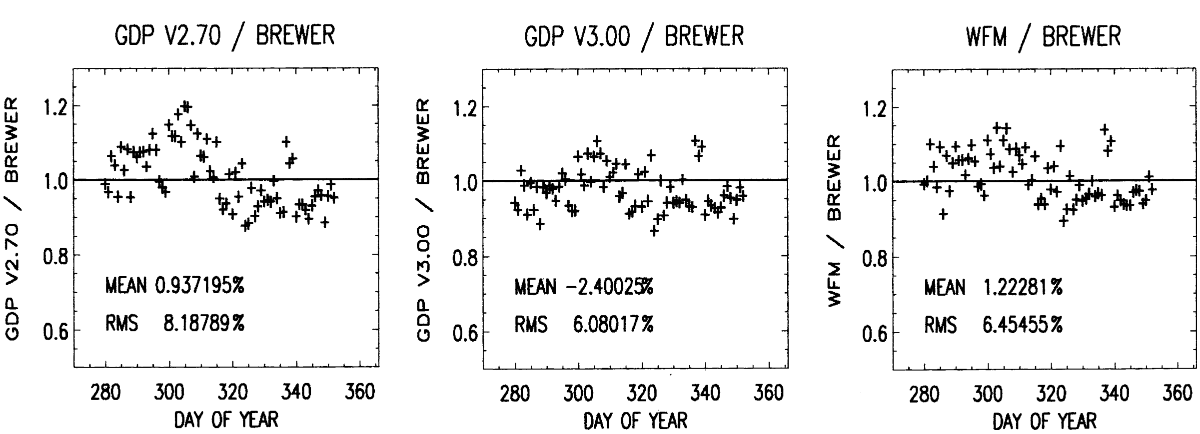

Fig. 4. Ratio of ozone column from GDP V2.70 (left) and GDP V3.00 (middle) to ozone column from Brewer measurements at Belgrano II Station. Right: ratio of ozone column from WFM-DOAS to ozone column from Brewer measurements.

when the AMF strongly varies with ozone absorption as in the case at large SZA.

Fig. 4 shows the comparison for Belgrano II Station. The overestimation of GDP V2.70 data compared to Brewer data under ozone hole conditions (until the beginning of November) and the underestimation in summer (late November and December) can be identified in the left panel. GDP V3.00 and WFM-DOAS tend to compensate these differences, less ozone in spring and enhanced ozone in summer, as shown in the middle and in the right panel. In spite of that, the seasonal behaviour is still present when comparing WFM-DOAS with Brewer data (right panel), but the RMS error is slightly reduced.

5. Conclusions and future work

Preliminary case studies have shown very promising results concerning the application of the weighting function modified DOAS algorithm for total ozone retrieval on synthetic data and GOME spectral intensities. Theoretical studies have shown its advantages as unknown atmospheric temperature can be retrieved simultaneously. The differences between satellite data and ground-based measurements can be reduced as demonstrated under ozone hole conditions at high polar latitudes. Compared to standard DOAS (GDP V2.70) the fit accuracy is significantly improved. GDP V3.00 and WFM-DOAS show similar ozone columns for Neumayer Station and Belgrano II, which is mainly due to the use of a better ozone profile climatology and the implementation of temperature fitting. Additionally, the weighting function approach takes the wavelength dependence into account, which is important for large SZA. The calculation of AMFs for standard DOAS requires the intensity with and without trace gas absorption. The linearization point in WFM-DOAS is a modelled intensity for a certain ozone scenario which is much closer to the real scenario than the standard DOAS intensity without ozone absorption.

Further investigations have to be performed concerning the optimum parameter spacing of the reference spectra look-up-table. The dependence on the relative azimuth angle has to be accounted for. Additional studies are planned to analyze the Ring effect on total ozone retrieval. Especially the influence of molecular Ring may be important under ozone hole conditions.

Acknowledgements

The authors thank the Alfred Wegener Institute for Polar and Marine Research and the Italian National Centre for Research for providing the ozone data. The GOME data were provided by European Space Agency through the German Aerospace Center (DLR). This work has been funded in parts by the German Atmospheric Research Program (AFO2000) under the guidance of BMBF and GSF (Project GOMSTRAT). We thank Andreas Richter for helpful suggestions with regard to DOAS issues and Michel van Roozendael from Belgian Institute for Space Aeronomy for providing his manuscript.

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