ON THE ACCURACY OF GOME AND SCIAMACHY TOTAL OZONE MEASUREMENTS IN POLAR REGIONS

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ABSTRACT

Total ozone retrieval algorithms applied operationally to GOME and SCIAMACHY data have been based on the Differential Optical Absorption Spectroscopy (DOAS) technique for several years. These algorithms produce retrieval results within the 1% precision level in low- and mid-latitude regions. However, in polar regions, there are persistent discrepancies with respect to reference ground-based and complementary satellite data sets (e.g. from the TOMS instrument).

We use the Direct Fitting part of the GODFIT software to investigate these total ozone retrieval issues in the polar regions. Sensitivity tests show the influence on the ozone columns of key input parameters such as cloud parameters (FRESCO or OCRA-ROCINN), O_3 climatology (TOMS v8 or DOC), surface albedo, and temperature profile data bases. The two SAUNA campaigns in Sodankylä (67° N, 26° E) provide good opportunities to validate our algorithm in polar regions. Based on these results, one expects a consolidation of the retrieved GOME and SCIAMACHY O_3 columns in polar regions, even at high solar zenith angle.

1. INTRODUCTION

The monitoring of the long-term trend of ozone and of its day-to-day variability is a key environmental task for our changing atmosphere. Since 1995, the ESA's Global Ozone Monitoring Experiment (GOME) [1] on board the ERS2 platform has been measuring the global distribution of atmospheric O_3 columns. Although global coverage was lost in June 2003 due to the failure of the tape recorder for intermediate data storage, the instrument is still in operation and provides high quality measurements above the Northern Hemisphere. Launched on board the ESA ENVISAT platform in March 2002, the SCaning Imaging Absorption spectroMeter for Atmospheric CartograpHY (SCIAMACHY) instrument [2] complements the GOME record, offering the potential for combined global total ozone data covering more than a decade. This of course requires appropriate assessment of the consistency between both instruments.

Version 4.0 of the operational Ground Data Processor (GDP 4.0) for GOME [3] is based on the GDOAS algorithm developed at BIRA-IASB which uses the Differential Optical Absorption Spectroscopy (DOAS) technique. Last year, a major revision of the operational SCIAMACHY processor (SGP 3.0) was realized at DLR-IMF [4]. Total O_3 columns from SCIAMACHY nadir UV/VIS measurements are again generated using an algorithm analogous to that at BIRA-IASB, adapted to the SCIAMACHY instrument (SDOAS). The first validation phase of this revision was done some months ago and a complete reprocessing of the SCIAMACHY data is expected soon. Operational processors for both instruments are similar, and a good consistency between their respective measurements is expected.

Validation exercises have shown that these two operational processors based on the DOAS technique lead to total O_3 columns with differences with respect to the ground-based measurements lower than the targeted 1% level in the low- and mid-latitude regions. However, in polar regions, correlative studies involving reference ground-based and complementary satellite data sets reveal larger differences, indicating persisting accuracy issues, both from space and ground-based measurements [5].

Within the ESA-funded GODFIT (GOme Direct FITting) project, the BIRA-IASB/RT-Solutions consortium has developed an advanced retrieval algorithm based on a direct fitting (DF) approach where backscattered spectral radiances simulated using the radiative transfer model LIDORT v2.5+ are fitted to measured radiances in a physical way [6]. In this paper, we present a variety of sensitivity tests performed using this retrieval algorithm, and we show the influence on retrieved total ozone columns of key input parameters such as the cloud parameters, the O_3 profile climatology, the surface albedo and the temperature profile data bases. Also, we will focus on the polar regions, and both SAUNA campaigns (March-April 2006 and February-March 2007) in Sodankylä (67°N, 26°E) have presented excellent opportunities to carry out these tests in high latitude and high solar zenith angles conditions.

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2. THE GODFIT ALGORITHM

To retrieve total ozone columns from satellite measurements, GODFIT uses a non-linear least-squares minimization procedure, which directly adjusts simulated radiances to the measured ones by fitting the elements in the state vector. The main difference with respect to the DOAS technique is the single-step nature of the fit: there are no intermediate products (slant columns and air mass factors).

Simulated radiances and weighting functions are calculated “on-the-fly” using the linearized radiative transfer model LIDORT in the forward model. The latter requires inherent optical property inputs (IOPs) constructed from key input parameters such as the O_3 cross-sections, the O_3 vertical profile, the temperature profile, the cloud parameters, and the surface albedo. The O_3 profile climatology has to be classified according to total O_3,, and the algorithm relies on a 1-1 correspondence between the fitted total column and the O_3 profile used in the radiative transfer. Each spectrum calculated with the forward model is then corrected for the molecular Ring effect. More details on the description of the algorithm itself are given elsewhere [6, 7]. Fig. 1 is an illustration of the total O_3 columns derived from GOME measurements between 1st and 3d April 1999 using GODFIT. The fitting window used for the O_3 retrieval lies between 325 nm and 335 nm.

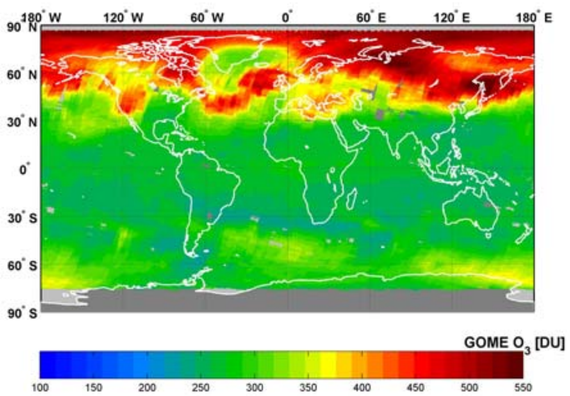

Figure 1. Total ozone columns retrieved from GOME measurements between 1st and 3rd April 1999 using the GODFIT algorithm.

3. THE OZONE CROSS-SECTIONS

The ozone cross-sections used in the DOAS operational algorithms for GOME and SCIAMACHY are respectively: the GOME FM 98 data [8] with an optimized pre-shift of 0.017 nm, and the Bogumil et al. data [9] with an optimized pre-shift of 0.020 nm and a +3% scale factor, the latter adjustment ensuring consistency between GOME and SCIAMACHY columns.

A fundamental difference between the operational algorithms and the GODFIT DF retrieval is that the effective temperature is adjusted in the DOAS retrieval procedure [3], while in GODFIT it is fixed at a value depending on temperature profile used in the simulations. In the framework of the first SAUNA campaign, the differences between the DOAS and DF results were mainly explained by the effective temperature differences (Fig. 2a-b). With different O_3 cross-section data sets for GOME and SCIAMACHY, the DOAS effective temperatures are different for the two instruments since each of the data sets has its own temperature dependence. Fig. 2b shows that the GOME FM 98 data lead to higher effective temperatures from the DOAS fitting than the effective temperatures originating from use of the Bogumil data; the latter are in quite good agreement with the values estimated from the temperature profile used in DF (see below). Consequently, the DOAS – DF discrepancies are dependent on the O_3 cross-sections used in the retrieval through their temperature dependence.

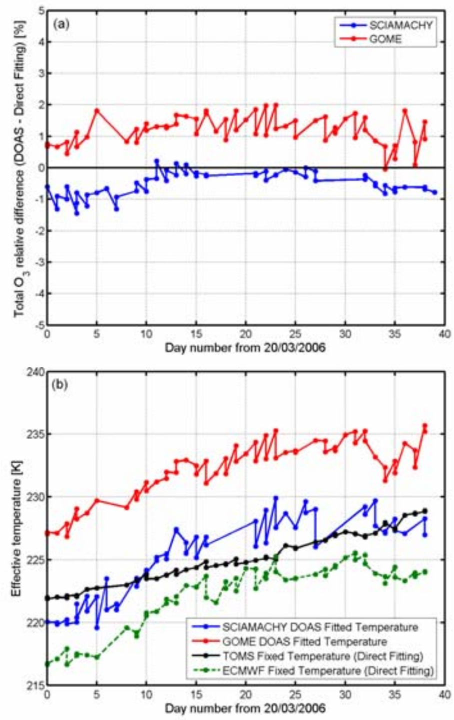

Figure 2. (a) Total ozone relative differences between the DOAS and Direct Fitting techniques for GOME and SCIAMACHY around Sodankylä during the first SAUNA campaign. (b) Comparison of the effective temperatures from the DOAS procedure using GOME FM 98 and SCIAMACHY Bogumil data, to the effective temperature estimated from the TOMS v8 or the ECMWF temperature profiles.

In order to have consistency between the two instruments, the same O_3 cross-sections should be used for both instruments (at the appropriate instrumental resolution). The high resolution Daumont and Malicet cross-sections [10] appear to be the optimal data set for ozone column retrieval using the DF technique in conjunction with a temperature profile taken from the ECMWF data. Indeed, they provide high quality fits for both GOME and SCIAMACHY; they give optimal consistency in terms of effective temperature retrieval (in DOAS scheme) and they lead to O_3 columns consistent with validated GDP 4.0 data.

4. SENSITIVITY TESTS

4.1. Temperature profile

First, temperature profiles required by the forward model were taken from the TOMS v8 climatology [11]. All profiles in this climatology are specified on an 11-layer pressure grid (which forms the current baseline in GODFIT), and they are binned monthly in 10° latitude bands. For each pixel, the required profile is obtained with bi-linear interpolation in latitude and time.

Recently, a new interface was implemented in the software in order to ingest more physically realistic temperature profiles from the ECMWF. The temporal and spatial resolutions are somewhat higher, as one profile is generated every 6 hours on a 1°×1° horizontal grid. The vertical resolution of these profiles is higher (37 layers), but currently we use the ECMWF temperatures interpolated to TOMS pressure levels. For each satellite pixel, the profile closest in time and place is selected.

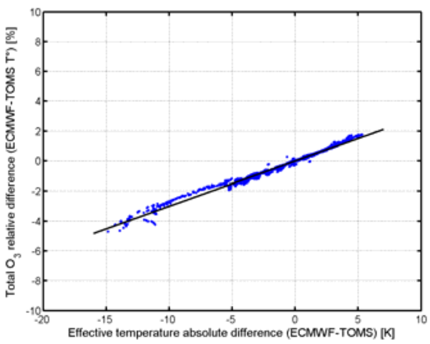

Figure 3. Total O_3 relative differences using the ECMWF temperature profiles or the TOMS v8 ones in the retrieval procedure of the GOME #23802 orbit versus the effective temperature absolute difference estimated from these two profiles.

For GOME #23802 orbit, Fig. 3 shows the influence of the temperature profile on retrieved total O_3 columns. Total O_3 relative differences are directly related to the absolute differences between effective temperatures estimated from the two profiles, via the temperature dependence of the O_3 differential cross-sections (about -0.3%/°K). Fig. 4 shows total O_3 relative differences due to the use of the ECMWF temperature profiles as opposed to the TOMS v8 profiles, for 24 GOME orbits in 1999. In general, differences vary between -1% and -2%, though they can reach -5% or +3% in some conditions.

The second SAUNA campaign in Sodankylä (67°N, 26°E) was organized in early 2007, and from Fig. 4, it is expected that differences between O_3 columns derived using the TOMS v8 T-profiles and those based on ECMWF ones will be significant. This is confirmed by Fig. 5, which shows these differences for SCIAMACHY retrievals around Sodankylä during this campaign. Fig. 5 also shows that the magnitude of these differences may quickly vary with time.

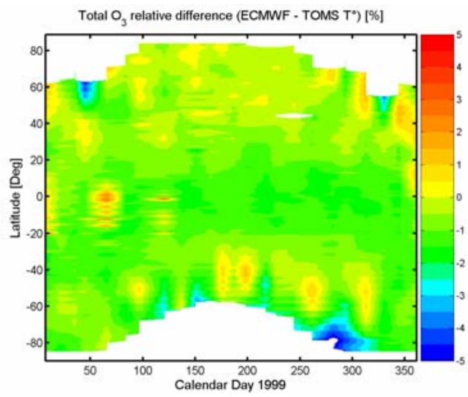

Figure 4. Total O_3 relative differences using the ECMWF temperature profiles or the TOMS v8 ones for 24 GOME orbits in 1999.

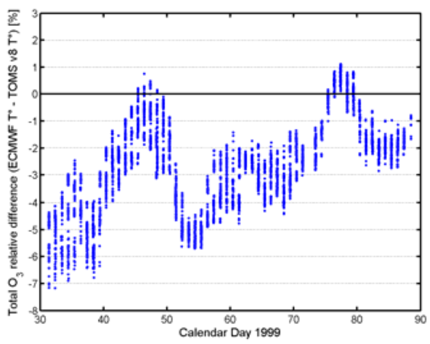

Figure 5. Total O_3 relative differences using the ECMWF temperature profile or the TOMS v8 ones for SCIAMACHY retrievals around Sodankylä during second SAUNA campaign (February-March 2007).

4.2. O_3 profile climatology

In order to highlight the influence of the O_3 profile on the retrieved total O_3 column, two column-classified climatologies were tested. The TOMS v8 climatology provides (for each month and 10° latitude band) profiles expressed as partial columns in [DU] for the 11 pressure layers. Secondly, the DOC climatology [12] gives VMR_{O3} and ρ_{O3} profiles for 61 altitude levels (from 0 to 60 km). These profiles are binned in

30° latitude bands and in six-month seasons (winter/spring and summer/fall), except for the tropics for which there is no seasonal distinction. For this comparison exercise, the DOC profiles were integrated in order to obtain the O_3 partial columns on the TOMS pressure grid. Currently, during the retrieval procedure, the spatially and temporally closest O_3-classified profiles are selected and a Lagrangian interpolation is then performed through these for the appropriate total O_3 column.

By comparing the total O_3 columns derived with these two climatologies for the GOME 24-orbit set (Fig. 6), we notice that the relative differences are strongly dependent on the latitude band and that they are most significant in the 30°-40° band. Indeed, the latter effect corresponds to the simultaneous transition from one latitude bin to another one in both climatologies.

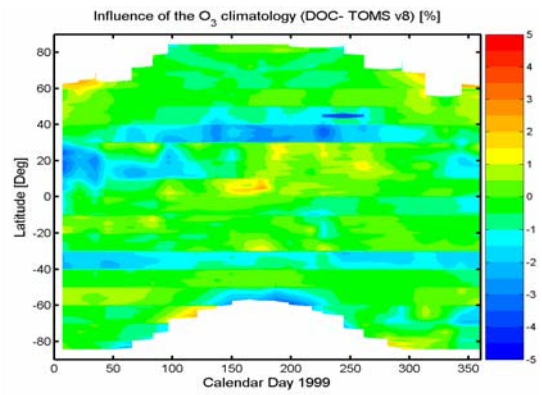

Figure 6. Latitude dependence of the total O_3 relative differences using the DOC and TOMS v8 climatologies in the retrieval procedure for 24 GOME orbits in 1999.

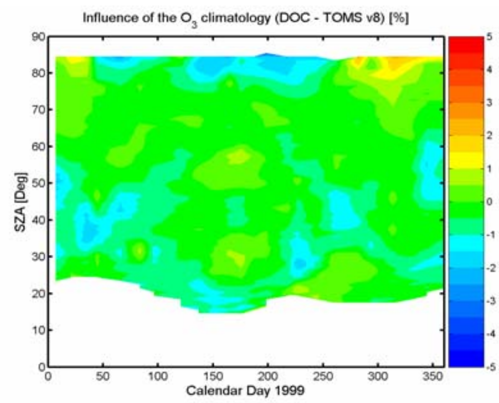

Figure 7. SZA-dependence of the total O_3 relative differences using the DOC and TOMS v8 climatologies in the retrieval procedure for 24 GOME orbits in 1999.

Fig. 7 and Fig. 8 show that the largest differences generally lie at very high SZA, highlighting the largest influence of the O_3 profile at low solar elevation on retrieved O_3 columns. Fig. 9 illustrates that relative differences are not constant in a latitude band for a given day since the climatologies are total O_3-classified and the retrieved columns are differently affected by the cloud coverage depending on the O_3 profile shape.

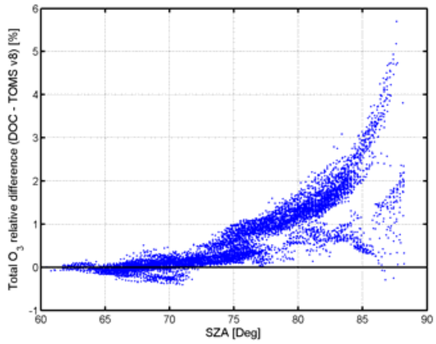

Figure 8. Total O_3 relative differences using the DOC and TOMS v8 climatologies for SCIAMACHY retrievals around Sodankylä during second SAUNA campaign (February-March 2007).

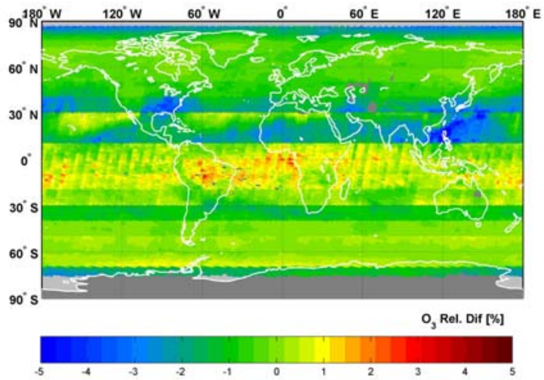

Figure 9. Total O_3 relative differences using the DOC and TOMS v8 climatologies in the retrieval procedure for the GOME orbits during 1-3 April 1999. Plotted differences are calculated as O_3(DOC)-O_3(TOMS).

4.3. Cloud algorithm

Cloud parameters used in the GODFIT software are generated by two different algorithms for the GOME instrument. The OCRA/ROCINN (v2.0) algorithm [13, 14] is fully integrated in the GODFIT code, and will generate cloud fraction (CF), cloud top albedo (CTA) and cloud top pressure (CTP). On the other hand, the FRESCO data [15] can be used as auxiliary input and gives for each pixel the CF and CTP while the CTA is set to 0.8. Both algorithms use an ice mode for pixels with high surface albedo; here, the CF is set to 1 and the CTA and CTP are generated. For SCIAMACHY, only FRESCO results can be used in GODFIT.

Fig. 10 (upper panels) compares the cloud parameters generated by both algorithms for normal mode (in blue) and ice mode (in red) pixels of 24 GOME orbits in 1999, and (lower panels) shows the effect of the parameter differences on the total O_3 columns. For normal-mode pixels, cloud fractional reflectivity (product of the CTA and CF) from FRESCO and OCRA/ROCINN are in quite good agreement even though the latter values are slightly larger. These cloud fractional reflectivity differences do not appear to be the main origin of the total O_3 relative differences, as there is no marked correlation between them. The cloud top pressures from both algorithms are also well correlated, but the dispersion is more significant and the FRESCO cloud top pressures are generally larger. The correlation between the O_3 relative differences and the CTP differences is more pronounced, indicating that the O_3 differences are directly related to the cloud height differences. Concerning the ice mode pixels, the OCRA/ROCINN cloud fractional reflectivities are generally smaller than the FRESCO values, thus giving rise to larger O_3 columns overall.

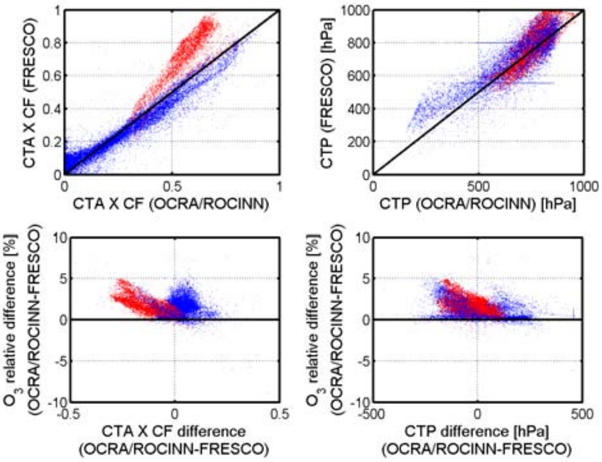

Figure 10. Upper panels: Comparison of the cloud parameters derived with FRESCO and OCRA/ROCINN for normal mode (blue points) and ice mode (red points) pixels; 24 GOME orbits in 1999. Lower panels: Influence of the cloud parameters on the total O_3 columns retrieved with GODFIT.

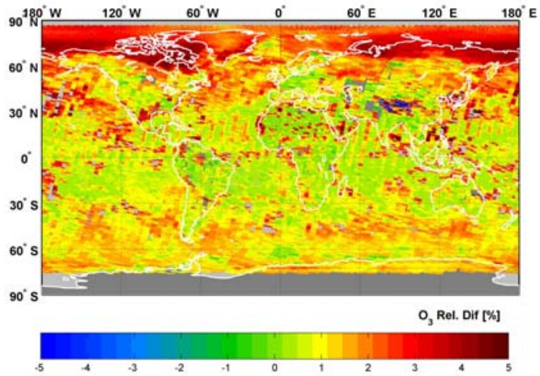

Figure 11: Relative differences in total O_3 for results generated with cloud parameters from OCRA/ROCINN and those based on FRESCO inputs, for GODFIT DF retrievals of GOME data for 1-3 April 1999. Plotted differences are calculated as O_3(OCRA/ROCINN) - O_3(FRESCO).

Fig. 11 shows that these cloud parameter differences lead to total O_3 differences generally lower than 2%. However, these differences are somewhat larger for the ice mode pixels, and can reach 4%.

4.4. Surface albedo

To highlight the influence of the surface albedo on the retrieved total O_3 column, air mass factors were calculated at 325 nm at different solar zenith angles for different surface albedo values using LIDORT. Fig. 12 shows the AMF relative differences due to surface albedo errors at different SZA. It can be seen that these relative differences increase linearly with albedo errors and are not very dependent on the SZA. Albedo uncertainties can then lead to significant error source on O_3 retrieval, even at low sun elevation.

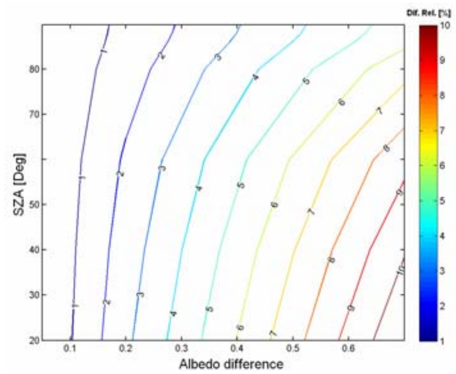

Figure 12. AMF relative errors [%] due to uncertainties in the surface albedo for different solar zenith angles .

5. CONCLUSIONS

In this work, the sensitivity of retrieved total ozone columns to a number of key input parameters was examined. First, use of ECMWF temperature profiles instead of those included in the TOMS v8 climatology may lead to important differences. As the DF retrieval contains no temperature adjustment, it is better to use the same O_3 cross-section data set for both GOME and SCIAMACHY in order to avoid inconsistent results caused by different cross-section temperature dependencies. The Daumont et al. data convoluted at the instrumental resolution lead to high quality fits and O_3 columns in good agreement with validated data.

By comparing the O_3 columns derived using the O_3 profile DOC and the TOMS v8 climatologies, it was observed that the sensitivity of the column is largest for high SZA (> 75°), and an appropriate choice of ozone profile is then crucial for the polar regions. However, these differences can also be non-negligible at lower SZA depending on the latitude, the total O_3 column and the cloud coverage.

Cloud parameter information used in the retrieval also affects the derived O_3 columns. We compared results based on the OCRA/ROCINN and FRESCO cloud algorithms. For most pixels, OCRA/ROCINN leads to slightly higher columns. Unfortunately, ozone column differences are far more marked for high albedo surfaces (the large majority of cases in polar regions).

Finally, we showed that the O_3 columns are almost as sensitive to surface albedo at high SZA than at low SZA. Uncertainties in the surface albedo may be quite important in polar regions where the albedo can change dramatically during seasonal turnover; potentially an important error source on the total O_3 columns.

The GODFIT project is currently in its validation phase, in which a lot of satellite vs. ground-based measurement comparisons will be performed, the focus is especially on polar regions. This should allow us to determine the best key input parameters to use for O_3 retrievals with the GODFIT software.

Acknowledgements

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