Diffuser plate spectral structures and their influence on GOME slant columns

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Technical note, January 2001

The problem

As soon as GOME spectra were available for analysis, several groups started to apply their own DOAS algorithms to derive slant columns of O_3 and NO_2, and later also BrO, OClO, SO_2, HCHO, H_2O and O_4. It soon became obvious, that the residuals obtained from the DOAS fit were not as good as expected from the SNR of the instrument, and that the residuals were not of random nature but systematic and rather stable over longer time periods. It turned out that using an earth-shine instead of the solar irradiance as a background improves the residual significantly, but this introduces the problem of an unknown amount of absorption in the background measurement. Several factors have been identified that contribute to the larger than expected residuals:

- The undersampling of the spectra in conjunction with the Doppler shift of the solar irradiance spectrum
- Small errors in the Ring spectrum
- Small variations in the effective slit function for not uniformly illuminated ground pixels

However, even with these effects considered, the quality of the residuals is poorer than expected.

A second but related problem became apparent when longer time series of NO_2 became available and could be compared with ground based measurements. While the general agreement between GOME and ground-based zenith-sky measurements is good, the **satellite data show much more variability** even at clean air sites (see Fig. 1), and **this variability is repeated in amplitude and phase almost identically from year for yea**r (see Fig. 3). Comparison between the operational product and scientific products from the University of Bremen and Heidelberg showed, that the effect is not restricted to the lv2-product but is reproduced by independent algorithms. Further analysis proved that the same problem exists for all other absorbers derived from GOME spectra, but with a specific pattern for each absorber and fitting window.

Why do we think that the diffuser plate is responsible for the problem?

In order to identify the source of the problem, several tests have been performed on GOME data as described below.

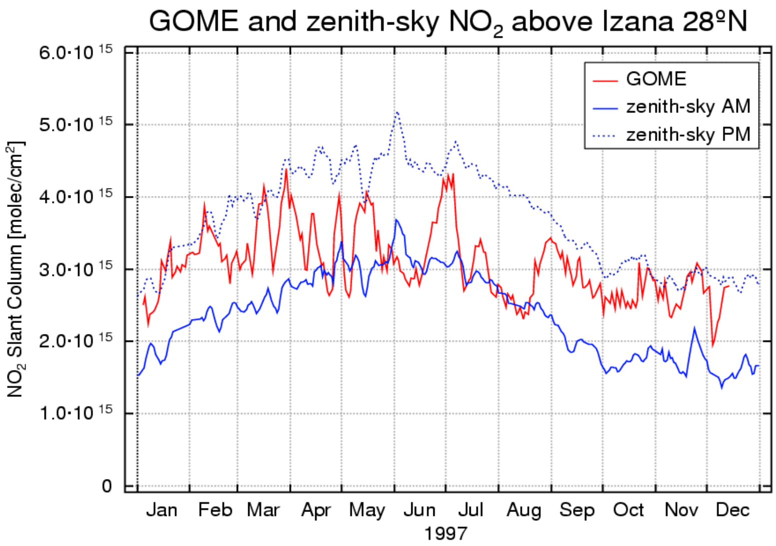


Figure 1: GOME operational NO_2 vertical columns above Izana as compared to ground based zenith-sky measurements (data courtesy of M. Gil and M. Yela). While the general values agree well, GOME columns show much more variability than expected, in particular in summer.

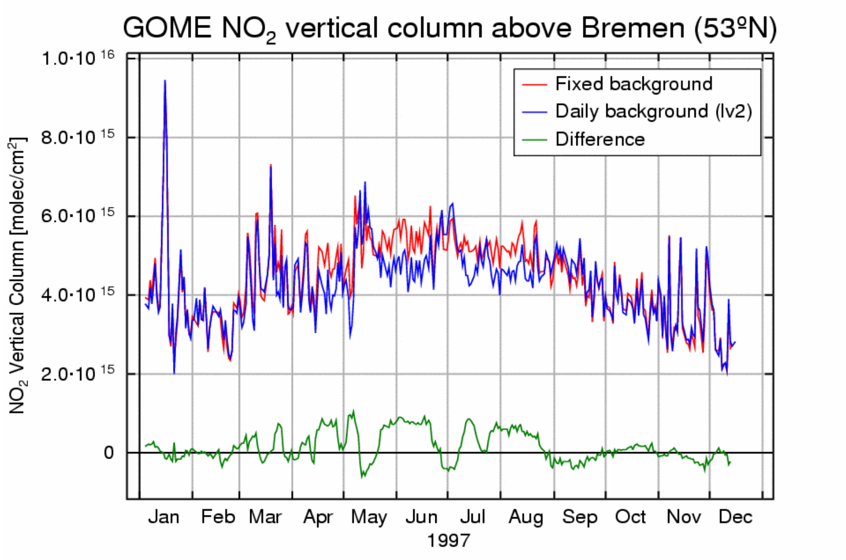


Figure 2: GOME NO_2 vertical columns above Bremen as derived with a daily irradiance spectrum (lv2 product) and a fixed background spectrum. The difference between the two evaluations is the structure introduced by the diffuser plate, but divided by the airmass factor applied to the slant columns.

First of all, a larger set of GOME data has been analysed using a single solar irradiance spectrum instead of the daily one. The resulting time series is much smoother and compares favourable to the ground-based measurements (Fig 2). However, the error cancelling achieved by using the daily irradiance spectrum is no longer in effect, and instrumental changes introduce drifts into the derived NO_2 time series. Also, the problem of what background spectrum to choose and thereby which offset to introduce to the slant columns remains unsolved. The fact, that the large variability seen in the lv2 data is not present in this special analysis shows, that **the problem lies with the solar spectra**, not with the earth-shine measurements.

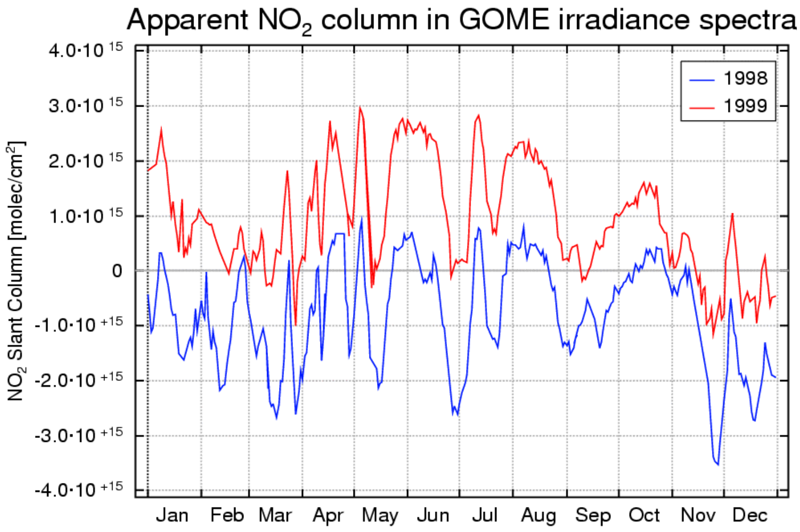


Figure 3: Apparent NO_2 slant column when applying the standard NO_2 fit to all GOME irradiance spectra, using one arbitrarily chosen solar spectrum as background. Small and random columns are expected, but large and systematic variations are found. The similarity between the structures found in this test and in Figures 1 and 2 are obvious.

In a second test, a large set of GOME irradiance measurements has been analysed for NO_2 absorptions using the same settings as in the standard NO_2 fit and an arbitrarily selected solar spectrum as background. The resulting NO_2 column should be very close to 0 and should not show any systematic structures. However, the fit retrieved large NO_2 columns (up to 3 10^{15} molec/cm^2) and a seasonal variation that matches the artifacts observed in the difference between GOME NO_2 and ground-based measurement (see Figure 3). From this result we conclude, that **the observed variation is introduced by variations in the solar irradiance measurement**.

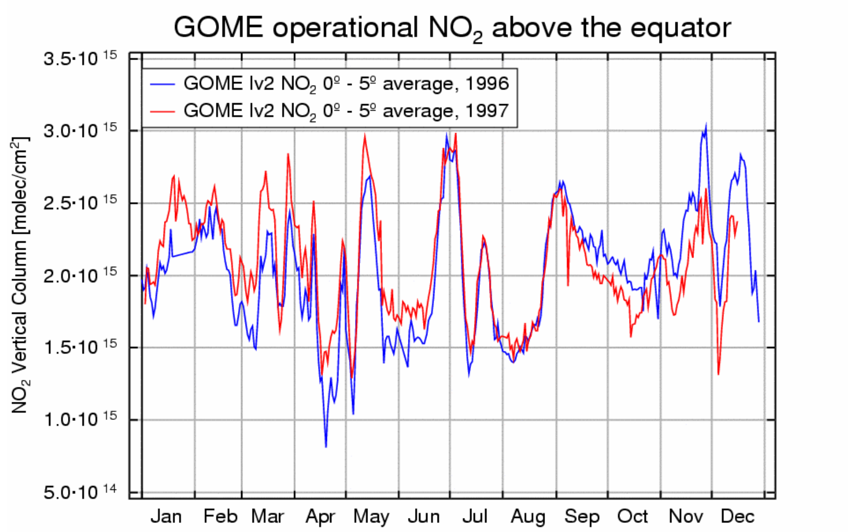


Figure 4: GOME operational NO_2 vertical columns above the equator for 1996 and 1997. Again, the structures seen in Figures 1-3 appear.

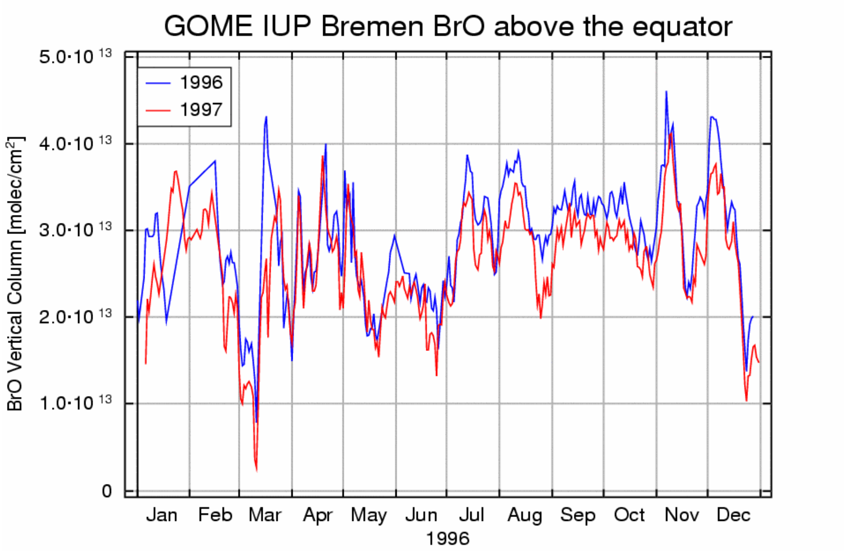
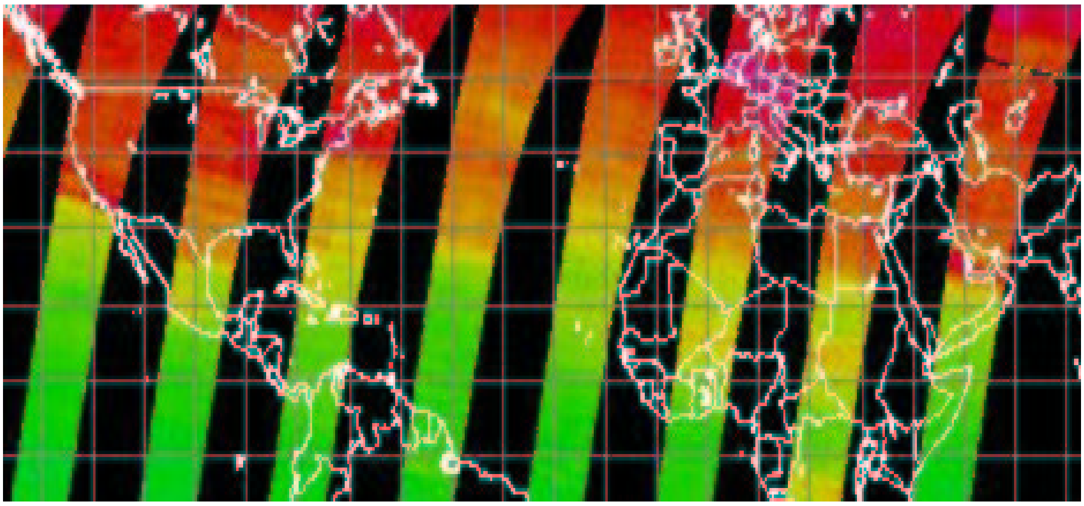
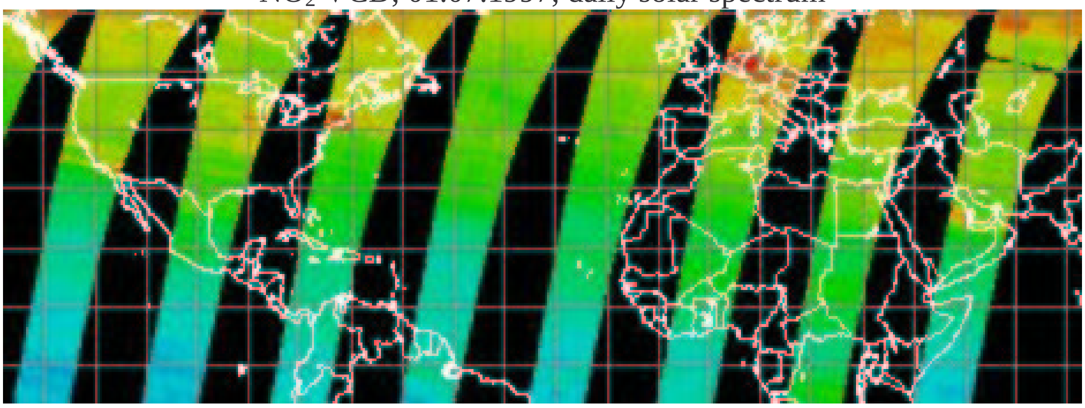


Figure 5: GOME BrO vertical columns above the equator for 1996 and 1997 as derived by the IUP Bremen. Again, similar structures seen in Figures 1 - 4 appear, however with a different amplitude and not at the same time of the year.



NO_2 VCD, 01.07.1997, daily solar spectrum



NO_2 VCD, 01.07.1997, fixed reference, solar spectrum from 01.01.1997

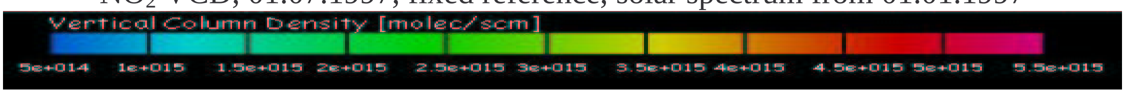


Figure 6: Examples GOME NO_2 maps for a day (01.07.1997) with a large uncertainty introduced by the spectral structures caused by the diffuser plate. Especially in the Tropics the difference between the evaluation with fixed or daily reference spectrum can be large (up to about 100%).

How large is the error introduced to the products?

The error introduced by the diffuser is a constant offset for slant columns derived using a specific irradiance spectrum and independent of location and solar zenith angle. The absolute error therefore depends on the airmass factor and the relative error on the vertical column to be expected. In general, the problem is most severe in equatorial regions and for small absorptions. In Figure 4, the slant columns integrated along the equator between 0° and 5°N latitude are plotted for two years for NO_2 (lv2-product), in Figure 5 the same exercise is shown for BrO. In this area, the relative **errors are up to 100% for NO_2** (see also Figure 6) and **70 – 100 % for BrO**, depending on what one assumes to be the true column. At higher latitudes, the relative errors are much smaller, but still significant as illustrated in Figure 2 for NO_2 above Bremen, where in summer errors of more than 20% are introduced . In general, the errors can only be neglected at high latitudes in winter or for scenarios with large absorptions such as OClO in the activated polar vortex, tropospheric BrO events in the polar regions or biomass burning scenarios.

What are possible solutions?

Three possible work-around solutions have been examined that could in principle eliminate the effect:

1. **Use of a single irradiance measurement as a background spectrum** for a longer time series. With this approach, the variations no longer are existent. However, instrumental changes introduce large drifts in the time series and also increase the fitting residuals with time. The method therefore gives acceptable results for NO_2 at mid- and high latitudes, but not for NO_2 at low latitudes and not for any one of the smaller absorbers (BrO, OClO, SO_2, HCHO). One general shortcoming of this method is that it remains open which solar spectrum yields the true absolute values.
2. **Use of selected earth-shine measurements as background spectrum**. With this approach, the unknown amount of absorption in the background spectrum has to be guessed and added to the derived columns. This is acceptable for OClO, where high sun scenarios with negligible OClO can be found in every orbit, but not for other absorbers where no such a priori knowledge is available.
3. For some absorbers the assumption can be made, that **concentrations in equatorial regions are constant and well known from models**, but this is difficult to justify and introduces noise and considerable uncertainty into the results. In addition, it by definition makes GOME measurements meaningless in tropical regions, one of the scientifically most interesting parts of the world.

All three methods have successfully been applied to certain questions but have large drawbacks and therefore should be avoided if possible.

Summary and conclusions

1. GOME irradiance measurements suffer from spectral artefacts, that correlate strongly with the differential absorption structures used for the retrieval of trace gases with the DOAS technique.
2. The variations introduced in the slant columns are independent of solar zenith angle and location, and are repeated from year to year.
3. The most probable explanation for the structures is a small angle dependence of the spectral reflectivity of the diffuser plate and the variation in the incident of solar radiation on the diffuser during one year.
4. The absolute error introduced by this effect depends on the molecule and the spectral region used for the retrieval and affects all absorbers. For equatorial regions it is of the order of 50% for NO_2, 75% for BrO and even more for weaker absorbers such as HCHO. With the exception of O_3, it is an important, if not the most important error source for all GOME columns at low and middle latitudes.
5. It also has to be pointed out, that with the diffuser structures, an uncertainty exists in what the *absolute* values are for all GOME products, as any choice of a specific solar irradiance spectrum will introduce its own slant column offset in the analysis.
6. There currently exists no satisfying algorithm or work around to compensate the effect for GOME data. All corrections applied to the fits or to the slant columns introduce other serious problems for the interpretation of the data.

We therefore conclude, that everything should be done to eliminate the source of the effect in the SCIAMACHY and GOME-2 instruments by introducing a diffuser with as little spectral characteristics as possible.