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# Effect of spectral structures on DOAS retrieval

## History

Action item on KNMI to investigate the effect of spectral structures similar to those of gaseous absorbers on the DOAS retrieval of $O_3$ (UV and VIS), $NO_2$, BrO and $SO_2$. This action originated from the OMI Instrument Preliminary Design Review (I-PDR), held at TNO-TPD, Delft in The Netherlands from 2 to 4 December 1998 and was formulated in Review Item Description (RID) NIVR-192 (originator P. Levelt).

This study replaces the draft version of 17 June 1999. Only a few minor corrections were made with respect to the draft version of 17 June 1999 (most important ones: the maximum error for the $O_3$ column is now 2% in stead of 1% and in Table 1, “Maximum dI” is corrected to “Maximum dI/I”).

## Description of the action

The effect on the DOAS retrieval is investigated of spectral structures similar to the absorption structures of the retrieved gases. The maximum value for these structures is calculated, for given error levels and slant column densities.

## Method

In the DOAS method the slant column density *scd* of a gaseous absorber is derived from the following formula:

$$-\ln\left(\frac{I_e(l)}{I_s(l)}\right) = f(l) + scd \cdot s(l)\,, \qquad (1)$$

where $I_e(l)$ is the earthshine radiance, $I_s(l)$ is the solar irradiance, $f(l)$ is a low order polynomial function and $s(l)$ is the absorption cross section for the given absorber. DOAS uses the fine spectral structure in the absorption cross section to derive the *scd*. Equation (1) can be rewritten as:

$$-\ln\left(\frac{I_e(l)}{I_s(l)}\right) = f'(l) + scd \cdot s'(l)\,, \qquad (2)$$

where $s'(l) = s(l) - g(l)$ and $g(l)$ is a polynomial fit of $s(l)$ of the same (or lower) order as $f(l)$. To investigate the effect of instrumental spectral features similar to those of the gaseous absorbers, $I_e(l)$ is perturbed with a signal with the spectral structure of $s'(l)$. This case reflects a worst case scenario. When the perturbation does not exactly fit the gas absorption structures, the effects on the DOAS retrieval are much smaller. For the perturbed radiance $I_e'(l)$ Equation (2) can be written as:

$$-\ln\left(\frac{I_e'(l)}{I_s(l)}\right) = f'(l) + scd \cdot s'(l) \cdot (1+e)\,, \qquad (3)$$

where $e$ is the systematic error in the retrieved *scd* due to the perturbation of the earthshine radiance.

Combining Equations (2) and (3) the error can be expressed in terms of the perturbation $dI(l)$.

$$\frac{dI_e(l)}{I_e(l)} = \left| \frac{I_e'(l)}{I_e(l)} - 1 \right| = \left| e^{(-scd \cdot s'(l) \cdot e)} - 1 \right| \approx \left| scd \cdot s'(l) \cdot e \right|, \tag{4}$$

Given a required maximum error $e$, the corresponding maximum value for $\frac{dI_e(l)}{I_e(l)}$ is computed by solving Equation (4) for the maximum value of $|s'(l)|$. It is noted that this also depends on the *scd*.

## Results

For $O_3$ (UV and VIS), $NO_2$, BrO and $SO_2$ the maximum amplitude of instrumental spectral structures can be computed from Equation (4). $s'(l)$ was computed by subtracting a second order polynomial function from $s(l)$. A third order polynomial was tested as well, but the differences with the second order polynomial were small. The maximum amplitude of $s'(l)$ was computed as half the peak-to-peak variation of $s'(l)$, see Table 1.

| | $O_3$ UV | $O_3$ VIS | $NO_2$ | BrO | $SO_2$ |
|---|---|---|---|---|---|
| Slant column density | 400 DU | 400 DU | $2 \times 10^{15}$ cm$^{-2}$ | $3 \times 10^{13}$ cm$^{-2}$ | $3 \times 10^{16}$ cm$^{-2}$ |
| Fit window [nm] | 320 – 335 | 450 – 500 | 425 – 450 | 345 – 360 | 314- 327 |
| Amplitude of $s'(l)$ [cm$^2$] | $4.7 \times 10^{-21}$ | $1.2 \times 10^{-22}$ | $1.7 \times 10^{-19}$ | $4.1 \times 10^{-18}$ | $3.0 \times 10^{-20}$ |
| Maximum error **e** [%] | 2 | 2 | 10 | 10 | 20 |
| Maximum dI/I | $1 \times 10^{-3}$ | $5 \times 10^{-5}$ | $3 \times 10^{-5}$ | $1 \times 10^{-5}$ | $2 \times 10^{-4}$ |

Table 1 Minimal detectable *scd*, fit window, amplitude of $s'(l)$, maximum error **e**, and resulting value of the amplitude *dI/I*.

As mentioned above, the error of instrumental spectral structures depends on the slant column density *scd*. To compute the maximum value of $\frac{dI_e(l)}{I_e(l)}$ for a given error level, the minimal expected *scd* or the minimal detectable *scd* should be used. For $O_3$ 400 DU is expected the minimum *scd*. For the other gases the detection limit for the GOME instrument is used. For $NO_2$ this limit is $2 \times 10^{15}$ molecules cm$^{-2}$ [*Burrows et al., 1999*]. For BrO and $SO_2$ the detection limit is estimated as $3 \times 10^{13}$ molecules cm$^{-2}$ ($1 \times 10^{13}$ molecules cm$^{-2}$ vertical column [*Richter et al., 1998*]) and $1 \times 10^{16}$ molecules cm$^{-2}$ (0.4 DU vertical column [*Eisinger and Burrows, 1998*]), respectively. For the maximum error the required accuracy as listed in Table 3.1 of the OMI-Science Requirements Document version 2 (SRD) was used.

Table 1 shows the maximum amplitude of instrumental spectral structures for the slant columns and error levels are also listed in Table 1. Instrumental spectral structures will give the largest problems for $O_3$ VIS, BrO, and $NO_2$ retrieval. Spectral structures of the order of $10^{-5}$ or smaller are needed not to exceed the maximum error. The same values for the maximum error are used for the UV as VIS windows in Table 1. The value for the maximum error for $O_3$ VIS (2%) is very strict. However, note that OMI does not intend to use the Visual channel for the retrieval of the $O_3$ column. For $O_3$ UV and $SO_2$ the effects of instrumental spectral structures on the DOAS retrieval are much smaller. For spectral structures of the order of $10^{-4}$ the maximum error is not exceeded.

## Conclusions

The effects on DOAS retrieval of an instrumental spectral structure was investigated for a worst case scenario when these structures exactly match the spectral features of the retrieved gases. The maximal tolerable error was set to the required accuracy. The maximum instrumental spectral structure was calculated for $O_3$ for retrieval in UV and VIS for the expected minimum slant column density, and for $NO_2$, BrO and $SO_2$ for minimal detectable slant columns reported for the GOME instrument. The effect is largest for O3 VIS, BrO and NO2, for which the spectral structures should be of the order of $10^{-5}$, or smaller. For $O_3$ UV and $SO_2$ the effects are smaller. The maximum amplitude of instrumental structures for these gases should be of the order of $10^{-4}$, or smaller. In practice, this means that instrumental structures with amplitudes smaller than $10^{-5}$ are tolerable. Structures with larger amplitudes should be investigated in the appropriate spectral windows.

## References

Burrows, J.P., and co-authors, *The Global Ozone Monitoring Experiment (GOME): Mission concept and first scientific results,* J. Atmos. Sci, 56, 151-175, 1999.

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