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Title: Spectral Knowledge Requirements for DOAS Products
Author: R.F. van Oss Checked: J. de Haan
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Spectral Knowledge Requirements for DOAS Products

History

This research was the result of an action item towards the OMI science team, raised during the OMI Instrument Preliminary Design Review (I-PDR), held at TNO-TPD, Delft in The Netherlands from 2 to 4 December 1998. The background of the issue was the difference between the Instrument Specification Document (RS-OMIE-0000-FS-021, version 1 of 22 June 1998) and the Science Requirements Document (RS-OMIE-KNMI-001, version 1 of 18 November 1998).

The relevant Review Item Descriptions (RIDs) were I-PDR NIVR-52 (originator J. Callies), I-PDR NIVR-84 (originator P. Levelt) and I-PDR NIVR-140 (originator P. Levelt), resulting in:

AI and/or RID description

The science requirement is that the spectral stability should be better than 1/100th spectral pixel, while the current design has a much lower stability.

Action item

AI on the science team to investigate if the requirement on the spectral stability of 1/100th pixel is really necessary or that this requirement can be relaxed to 1/50th pixel.

In forthcoming meetings between the OMI industry and the OMI science team, it was recognised that action mentioned above applies to the spectral knowledge (after software correction), while spectral stability refers to the mechanical and thermal stability of the instrument (which introduces interpolation errors when co-aligning Earth radiances and solar irradiance spectra).

The I-PDR action item was replaced by several new actions, which can be summarised in the following action:

KNMI to test what are the spectral requirements on the wavelength grid for ozone profile and DOAS retrieval and define it in terms of two separate requirements: a **mechanical and thermal stability** requirement and in a **spectral knowledge** requirement.

This study focuses on the spectral knowledge requirements of the DOAS products and replaces the draft version "Spectral stability - Consequences for DOAS retrieval" of 11 June 1999.

The spectral knowledge requirements for the ozone profile are described in RS-OMIE-KNMI-226 (version 1, in preparation) and the mechanical spectral stability requirements are described in SN-OMIE-KNMI-203 (version 3 of 7 December 2000).

Description of action

The effect of an error in the wavelength registration of 1/50th and of 1/100th CCD- pixel in the level 1b OMI spectra on the DOAS slant column density retrievals of Ozone (UV and VIS), NO₂, SO₂, and BrO has been studied.

The method employed here is an "end-to-end" calculation. This means that OMI level 1b spectra are simulated using a radiation transfer model and an instrument model. Distorted spectra, containing errors in the wavelength registration, as well as undistorted spectra are generated. On these simulated spectra slant column densities are retrieved using the DOAS method. In this way, the errors on the slant column resulting from errors in

wavelength registration are determined. The effect of an erroneous spectrum is established for a number (16) of cases, differing in ground albedo, solar zenith angle, viewing angle and vertical column density of the gas. These cases cover the range of realistic parameter values relevant for the OMI observations.

The spectra are calculated for a mid-latitude summer standard atmosphere. The concentrations of gasses, other than the one under consideration, have been set to zero. The vertical column of the gas is tuned by a multiplication factor that is constant with height. For the radiative transfer calculations, MODTRAN (version 3.7) was used. The spectral resolution of MODTRAN is sufficient in view of the slit function of OMI.

The DOAS fit is employed using only the absorption spectrum of the gas. Since the perturbation only affects the slant column density and not the air mass factor, the effect on the slant column density is calculated.

Table 1 summarises the details of the radiation transfer model.

Table 2 summarises the details of the OMI instrument model.

The instrument simulation involves (i) the convolution of the calculated high-resolution spectrum with a (nearly Gaussian) slit function, (ii) the sampling of the radiances on the instrument wavelength grid and (iii) adding noise using a Gaussian random generator. The noise amplitude is calculated including only shot noise and electronic & detector noise (Ref b). A co-adding factor is used. For the present purposes this factor has been given an unrealistic high value (1e6) to make the noise artificially low to be able to detect small changes in the radiance and the resulting DOAS columns. Simulations with a more realistic noise level will not change the magnitudes of the consequences of the wavelength distortions, only that small consequences can not be detected anymore.

Table 3 presents the 16 cases used for the calculations.

Table 3a gives the vertical column densities.

The SO₂ low column density is based on the reported threshold for GOME (Eisinger & Burrows, ESAMS Scientific Sessions, ESTEC, Jan. 1999) (Ref. (e))

Table 4 presents for each gas the channel and wavelength region used and the details of the errors in wavelength registration (“shift or squeeze”) that have been introduced in the simulated spectra.

The wavelength ranges used for the DOAS fit are chosen identical to those used for GOME retrievals. Note that other ranges could be more suitable for OMI.

The shift (in nm) represents a constant wavelength perturbation, $\pm 1/50$ and $\pm 1/100$ pixel are used. The squeeze leaves the central wavelength in the window unchanged but results in a wavelength shift, which is linear in distance from the center. The magnitude of the squeeze is such that at the boundaries the wavelengths change an amount $\pm 1/50$ or $\pm 1/100$ pixel.

*Definition: $wl := wl_center + (wl - wl_center) * squeeze + shift$,*

The shift and squeeze are always employed separately.

The shifts and squeezes are only applied to the earthshine spectrum and not on the solar spectrum. This has more severe consequences for the retrieval compared to an equal shift for the sun and the earth spectrum, but it is nonetheless a realistic error.

A total of eight perturbed spectra are produced resulting from four shifts and four squeezes.

Results

In Figure 1 the perturbations of the slant column density are shown, defined as:

$$\text{Perturbation} = 100\% * (N_{dis} - N_{undis}) / N_{undis}$$

with N_{dis} the slant column derived from the distorted spectrum and N_{undis} the slant column from the undistorted spectrum.

Conclusions and discussion

The effect on the slant column density of a relative wavelength shift between the earthshine and the solar spectrum depends critically on the specie and the wavelength range used in the DOAS fit.

O₃ UV:

The effect on the slant column is less than 0.6 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 0.3%.

O₃ VIS:

The effect on the slant column is less than 5 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 2%.

NO₂:

The effect on the slant column is less than 10 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 5%.

BrO:

The effect on the slant column is less than 8 % for a wavelength distortion of 1/50th pixel.
For 1/100th the effect is less than 5%.

SO₂:

The simulated spectra of the low vertical column density appeared to be extremely sensitive to wavelength shifts and squeezes. For the low column (GOME threshold), the effect on the slant column reaches up to 520% for a wavelength distortion of 1/50th pixel. For 1/100th the effect is 270%. For the high vertical column density the effect on the slant column reaches up to 75% for a wavelength distortion of 1/50th pixel. For 1/100th the effect is 30%. We note that for a more realistic model which includes O₃ and SO₂ a somewhat higher accuracy may be required.

When we compare the effect of the wavelength distortions on the slant column to the requirements on the accuracy listed in Table 3.1 of Ref (c), the following conclusions can be drawn.

For Ozone UV (Req: 2 %), NO₂ (Req: 10 %) and BrO (Req: 10 %) a stability of 1/50th CCD-pixel is barely enough to satisfy the requirement. If the wavelength grid is stable up to 1/100th of a pixel the requirements can be safely met.

For Ozone VIS even a stability of 1/100th pixel is not enough to meet the required accuracy.

For SO₂ (Req: 20 %) the spectral stability of 1/100th pixel is even for the high column density (10x GOME threshold) not good enough to ensure the required accuracy.

Note that this report only discusses the effect of the spectral knowledge on the slant column. Since the noise level has been turned artificially low, a more realistic noise level will result in an even more reduced accuracy.

References

- (a) Information for the industry needed to close RIDs of the OMI Preliminary Design Review meeting at TNO/TPD in Delft on December 2-4, 1998, KNMI-FAX of 5 March 1999
- (b) Van der A, R., Noise levels of OMI instrument, personal communication, Jan 1999
- (c) Science Requirements Document for OMI-EOS, RS-OMIE-KNMI-001, V. 2-draft of 22 August, 2000.
- (d) Kruizinga, B., Radiometric effects of remnant polarisation in OMI due to the polarisation scrambler, Jan 1999, TNO-TPD
- (e) Eisinger, M. and J.P. Burrows, *GOME observations of tropospheric sulphur dioxide*, in proceedings ESAMS'99 European Symposium on Atmospheric Measurements from Space, ESTEC, Noordwijk, The Netherlands 18-22 January 1999, ESA WPP 161 ISSN 1022-6656, p. 415-419, March 1999.

Table 1: Atmospheric and observational parameters

Radiation transport model	MODTRAN version 3.7
Spectral sampling	5 cm ⁻¹ (= 0.08 nm at 400 nm)
Multiple scattering	DISORT 8 stream
Solar irradiance spectrum	Kurucz, 1 cm ⁻¹ tabulation, 5 cm ⁻¹ resolution
Atmospheric profiles of constituents	Mid Latitude summer, with constant factors to adjust columns of selected gasses (Tbl. 3)
Albedo	0.2 or 0.8, Lambertian (Tbl. 3)
Aerosol model	No aerosols
Solar zenith angle	20° or 80° (Table 3)
Viewing zenith angle	180° or 130° (Table 3)
Wavelength range	Specific for gas (Table 4)

Table 2: Instrument model

Slit function	tabulated slit function (GOME instrument model)															
Resolution	Channel 1: 1.00 nm Channel 2: 0.45 nm Channel 3: 0.63 nm															
Spectral sampling	Channel 1: 0.32 nm Channel 2: 0.15 nm Channel 3: 0.21 nm															
Channel bounds	Channel 1: 270 – 314 nm Channel 2: 306 – 380 nm Channel 3: 350 – 500 nm															
Noise	Noise (rms) = C * sqrt(S/C + N*N)/SQRT(co-adding) (co-adding = 1e6) With: S signal in photon/(s*sr*cm ² *nm) Noise in photon/(s*sr*cm ² *nm) N, C depend on channel: <table border="1" style="margin-left: 40px;"> <thead> <tr> <th></th> <th>N</th> <th>C</th> </tr> </thead> <tbody> <tr> <td>Channel 1A</td> <td>30</td> <td>1.47e7</td> </tr> <tr> <td>Channel 1B</td> <td>260</td> <td>1.47e7</td> </tr> <tr> <td>Channel 2</td> <td>260</td> <td>8.97e7</td> </tr> <tr> <td>Channel 3</td> <td>260</td> <td>3.15e8</td> </tr> </tbody> </table> Channel 1A < 300 nm, Channel 1B > 300nm		N	C	Channel 1A	30	1.47e7	Channel 1B	260	1.47e7	Channel 2	260	8.97e7	Channel 3	260	3.15e8
	N	C														
Channel 1A	30	1.47e7														
Channel 1B	260	1.47e7														
Channel 2	260	8.97e7														
Channel 3	260	3.15e8														

Table 3:

Case	Solar zenith angle	Viewing zenith angle	Albedo	Column density ¹⁾
1	20°	180°	0.05	low
2	80°	180°	0.05	low
3	20°	180°	0.80	low
4	80°	180°	0.80	low
5	20°	130°	0.05	low
6	80°	130°	0.05	low
7	20°	130°	0.80	low
8	80°	130°	0.80	low
9	20°	180°	0.05	high
10	80°	180°	0.05	high
11	20°	180°	0.80	high
12	80°	180°	0.80	high
13	20°	130°	0.05	high
14	80°	130°	0.05	high
15	20°	130°	0.80	high
16	80°	130°	0.80	high

1) See Table 3a

Table 3a

	High column density	Low column density
O3 UV/VIS	501 DU	167 DU
NO ₂	(0.4 DU) $1.2 \times 10^{16} \text{ cm}^{-2}$	(0.2 DU) $5.9 \times 10^{15} \text{ cm}^{-2}$
BrO	$1.3 \times 10^{14} \text{ cm}^{-2}$	$6.3 \times 10^{13} \text{ cm}^{-2}$
SO ₂	(5.6 DU) $1.5 \times 10^{17} \text{ cm}^{-2}$	(0.6 DU) $1.5 \times 10^{16} \text{ cm}^{-2}$

Table 4

	O ₃ -UV	O ₃ -VIS	NO ₂	BrO	SO ₂
Channel	2	3	3	2	2
Wavelength range [nm]	325 – 335	450 - 500	425 – 450	345 - 360	314 – 327
Shift [nm]	±0.003	±0.0042	±0.0042	±0.003	±0.003
	±0.0015	±0.0021	±0.0021	±0.0015	±0.0015
Squeeze [-]	1.0006, 0.9994	1.000168, 0.999832	1.000336, 0.999664	1.0004, 0.9996	1.00046, 0.99954
	1.0003, 0.9997	1.000084, 0.999916	1.000168, 0.999832	1.0002, 0.9998	1.00023, 0.99977

Figure 1: Perturbation in slant column density resulting from 9 perturbations in the simulated OMI level 1 spectra for 16 cases. a: O3UV, b: O3VIS, c: NO2, d: BrO, e: SO2.





