OMI in-flight wavelength calibration and the solar reference spectrum

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Abstract

The Ozone Monitoring Instrument (OMI) was launched in July 2004 and is one of four instruments onboard NASA's EOS-Aura satellite. OMI is a nadir-viewing UV-VIS spectrometer ranging from 270 to 500 nm, with a spectral resolution of roughly 0.5 nm. OMI obtains daily global coverage at the equator with a nominal sampling at nadir of 13x24 km^2.

This paper discusses the in-flight wavelength calibration and the solar reference spectrum. Wavelength calibration is performed by means of fitting Fraunhofer structure in the radiance and irradiance spectra. It was found that when observing rapidly changing radiance signals, the wavelength scale changed in tune with this. We describe the details of this effect, explain the underlying optical mechanism and show that we can (and do) correct for it with a high degree of accuracy. This effect will be observable in any spectrometer with similar optics as that of OMI.

A prerequisite for any in-flight wavelength calibration method that uses Fraunhofer lines in the observed spectra is a good quality high resolution solar reference spectrum. We describe how we calculate such a spectrum, based on combining high resolution ground based data, and medium resolution satellite measurements.

1 The Ozone Monitoring Instrument

The ozone monitoring instrument (OMI) is one of four instruments aboard the EOS-Aura satellite and is the result of a collaboration between Dutch and Finnish institutes. Aura was launched successfully on 15 July 2004 and orbits the Earth in a Sun-synchronous orbit at an altitude of about 700 km, passing the equator northward at 13.42 local time. The Aura mission is to observe the Earth's atmosphere in order to answer questions concerning the possible recovery of the ozone layer, air quality and the changing climate. OMI contributes to these mission objectives in all those fields. OMI is an ultraviolet-visible spectrometer with a wide instantaneous field-of-view perpendicular to the flight direction. Using the OMI measurements a number of atmospheric trace gases can be studied, as well as aerosols and clouds. For Ozone, NO_2, SO_2 and various minor trace gases the total columns are retrieved for small ground pixels (at nadir: 13 km x 24 km). In addition, ozone profile information for the same ground scenes (at 13 km x 48 km resolution) is retrieved. OMI is a successor to instruments like the GOME, TOMS, SBUV and SCIAMACHY.

OMI measures the Earth radiance and the Sun irradiance. Most of the retrieval algorithms use the Sun light that is scattered from the Earth and its atmosphere as the main input for their retrievals. Scattered Sun light that enters the instrument is reflected off two telescope mirrors that project an image on the entrance slit of the spectrograph. The spectrograph is divided into two spectral channels: a UV and a VIS channel, that cover the wavelength ranges 270-370 nm and 350-500 nm, respectively. In order to suppress stray light, the UV channel is divided into two sub-channels at about 310 nm: UV1 and UV2. The spectral sampling and resolution are different for the different channels: UV1: 0.33/0.63 nm, UV2: 0.14/0.42 nm, VIS: 0.21/0.63 nm, respectively. The instantaneous field of view in the flight direction is about 1.0 degree, which corresponds to about 10 km on the ground. In nominal operational mode, the information in the across track direction is binned to 60 ground pixels in the UV2 and VIS channels and 30 in the UV1. In the flight direction, images are co-added to restrict the data rate. Typically two to five individual exposures (depending on the expected radiance levels) are co-added.

The UV and VIS channels have separate CCD detectors of 780 pixels by 576 pixels, in the spectral and across-track direction, respectively. For one column (wavelength) per CCD detector the individual read-outs are retained. These are the so-called small-pixel column radiances. These small-pixel column radiances are therefore available at a 2-5 times higher frequency than the complete images, and for that reason they allow to see structures on the ground or in the atmosphere with a higher spatial sampling. The small-pixel columns were originally included in the design to study the effect of clouds. They will play a crucial role in the in-flight wavelength assignment, as will be described in this paper. More details on the OMI instrument can be found in [1,2].

2 Wavelength Calibration with OMI: scene dependence.

From scientific sensitivity studies it was determined that the required in-orbit accuracy of the wavelength scale is on the order of 1/100th of a pixel, which is ten times better than can be achieved by using a line lamp spectrum. This accuracy can be reached by using the solar Fraunhofer absorption lines in the Earth spectra. This method has also been employed in previous satellite missions [3]. The basis of the method is a high resolution solar reference spectrum (see next section). This reference spectrum is convolved with the instrument transfer function (spectral slit function) in order to obtain a simulated OMI solar measurement. The wavelength scale of this spectrum, at the instrument's resolution has the same accuracy as that of the original high resolution spectrum, provided the slit function is well known. For OMI the spectral slit functions as a function of viewing angle and wavelength have been accurately calibrated on the ground by use of a purpose-built optical stimulus that utilizes an echelle grating [4]. Thus, we are confident that the accuracy of the wavelength scale of the convolved spectrum is comparable to that of the original solar reference spectrum.

The original wavelength scale of a solar measurement is adjusted so that it matches that of the convolved solar reference spectrum at OMI resolution. For Sun light scattered from the Earth and its atmosphere the same method is employed in principle, but in addition to the Fraunhofer lines, the Earth reflected spectra also contain spectral structure originating from absorption and scattering that takes place in the Earth's atmosphere. The most important additional spectral structures are produced by Ozone and by inelastic scattering, or the Ring effect [5,6]. When performing the wavelength calibration of an Earth reflected spectrum, we fit an optimal linear combination of these contributions, using a non-linear solver based on a Levenberg-Marquardt algorithm.

The wavelength scale is known to vary with the temperature of the optical bench of OMI. The temperature dependence was studied pre-flight and found to be small, typically 0.01 pixel shift per Kelvin. With a temperature change over an orbit of at most a few tenths of a Kelvin, this results in a change of a few 1/1000th of a pixel. Before launch the wavelength scale was expected to vary mainly as a result of these temperature changes, so the wavelength scale was anticipated to be highly stable in-flight. With this in mind, as well as the considerable computational cost of performing wavelength calibration calculations for each individual spectrum and viewing angle, it was decided to calculate the wavelength scale for each spectrum based on the wavelength scale given at a reference temperature (based on the wavelength calibration of a large number of solar spectra obtained at the reference temperature of 264 K) and the correction based on the temperature of the optical bench. Thus, the wavelengths are *assigned* (predicted) rather than *calibrated*.

In the L1B product the wavelength scale is described by a polynomial rather than given for each sampled point. So, for each channel (UV1, UV2, VIS) and for each row in the measurement, the wavelength for column x is given by

$$\lambda = \sum_{i=0}^{n} c_i \left(x - x_0\right)^i \qquad (1)$$

where x is the pixel number, x_0 is a reference column, c_i the polynomial coefficients for the i-th order and n the order of the polynomial, which is four for all channels.

2.1 In-flight variability

When the first spectra came in, it became clear that the wavelength scale does not vary smoothly over an orbit, as would be expected from the observed temperature changes. Moreover, the amplitude of the wavelength variations is much larger than expected, up to half a pixel. The observed variations do not correlate with changes in the temperature of the OMI optical bench and the wavelength shifts induced by the temperature change are about two orders of magnitude smaller than the observed wavelength shifts. If these observed variations are not accounted for, the error in the predicted wavelength scale of the calibrated radiance product would be on the order of a few tenths of a pixel, which is in strong disagreement with the requirement of 1/100th of a pixel. In turn, such an error would lead to unacceptably large errors in higher level products such total column ozone, NO_2 and SO_2. Further investigation revealed that the rapid changes in the wavelength scale correlate with rapid changes in the observed ground scene radiances. Such changes often occur near clouds and near snow and ice boundaries.

The findings described above can be understood by taking a closer look at the optics of the OMI instrument. The way the spectrograph images a monochromatic narrow beam on the CCD detectors is described by the so-called spectral slit function. Both the shape and the width of the spectral slit function were accurately determined on the ground for all wavelengths and all viewing angles. The exact shape of the slit function has an immediate effect on the wavelength calibration. The spectral slit function was found to exhibit some degree of asymmetry. If instead of this real asymmetric slit function a symmetric slit function of the same width is assumed, the wavelength scale of the solar reference spectrum (i.e. the high resolution solar spectrum convolved with the OMI slit function) can change by as much a 0.03 nm. And since the wavelength scale of the solar reference spectrum determines the wavelength scale of all OMI measurements, this has a non-negligible impact. When the observed ground scene does not fill the spectrometer's entrance slit homogeneously in the flight direction, for example in the case of clouds, the shape and the position of the maximum of the spectral slit function change. The OMI instantaneous field of view in the flight direction is 1.0 degree, corresponding to about 10 km on the ground, which is a typical size for clouds. The change in shape and position of the spectral slit function subsequently leads to an observed shift in the wavelength mapping of the solar Fraunhofer lines on the CCD detectors. These are the wavelength shifts that we observe in the Earth measurement data as clouds move in and out of the field of view in the flight direction.

It must be noted that the above mechanism is not typical for OMI alone, but can also play an important role in other hyperspectral Earth observation spectrometers with comparable resolution and field-of-view size. However, scanning spectrometers like GOME and SCIAMACHY will suffer less from this mechanism since they scan a much larger ground scene. This has an averaging effect on the observed shifts, which intrinsically limits the accuracy of the wavelength calibration accuracy.

2.2 Correcting for the observed wavelength shifts

During a co-added (typical co-adding factor 2-5, see above) OMI measurement the radiances of the observed scene may vary quickly, mostly due to scattering by clouds. Fortunately, for nearly all of the recorded spectra, we have knowledge of the radiance history during one complete co-addition period, by means of the small pixel column radiances. These can be used to predict the change in the wavelength scale. As indicated above, there is a strong correlation between the observed change in wavelength scale and the relative change in radiance *between two subsequent measurements*. By use of the small pixel radiances we can actually see what happened *during the measurement itself,* because the small-pixel column radiances are available at a higher time resolution than the complete images. The use of these data leads to even higher correlations (mostly between 0.9 and 0.99) between the relative change in signal and the observed wavelength shift. The correlation factor is high, but the scaling between the two signals is dependent on wavelength and viewing angle.

The next step is to use these dependencies to come to a better in-flight determination of the wavelength scale. For each wavelength (column) and viewing angle (row) we calculate the factor needed to convert the observed rate of change in radiance to an equivalent shift in wavelength in nm:

$$\Delta\lambda(row,col) = F(row,col)\cdot\Delta rad(row,col) \qquad (2)$$

where $\Delta\lambda$ is the shift in wavelength in nm, F the conversion factor and Δrad the observed rate of change in the small pixel column radiance. These conversion factors are different for the different channels.

With these conversion factors for the UV2 and VIS channels we can correct the wavelength scale using the observed rate of change of the small pixel column radiance. In Fig. 1 we show how well this correction works. The top left of the four panel plot shows the relative change in the first wavelength polynomial coefficient for the VIS channel for orbit 3499. The top right shows the relative change in radiance multiplied by the pre-calculated conversion factor. The bottom left panel shows the difference of the two top panels. The bottom right plot shows the observed shift (Delta Calibration) *versus* the pre-calculated shift (Delta Assignment).

For the UV1 channel there is no clear correlation between the observed wavelength shift and the relative change in the radiance (correlation coefficient < 0.2). The reason for this is that at these short wavelengths (<310 nm) light is reflected high in the atmosphere, well above the Earth's surface and the majority of the clouds. This means that relative changes in the radiance are much smaller at these wavelengths than e.g. in the VIS channel. As a result the variability of the wavelength scale during an orbit is also much smaller. In fact, it is smaller than the scientific requirement on the accuracy in that channel, which is $1/50^{th}$ of a pixel. Thus, there is no need to correct the wavelength scale in the UV1 channel. So, the wavelength scale of the UV1 channel is left unchanged after the initial wavelength assignment step.

We note that the difference between calibration and assignment (Fig. 1, bottom left) is only an indication for how well the correction works, but it is not a direct measure. The reason for this is that the wavelength calibration itself is not infinitely accurate. In the VIS channel the wavelength calibration is expected to be highly accurate, but in the UV channel, especially at high solar zenith angles, the effect of Ozone on the signal, and therefore on the wavelength calibration becomes noticeable. The results shown in Fig. 1 are representative for all orbits and all viewing directions in the UV2 and VIS channels.

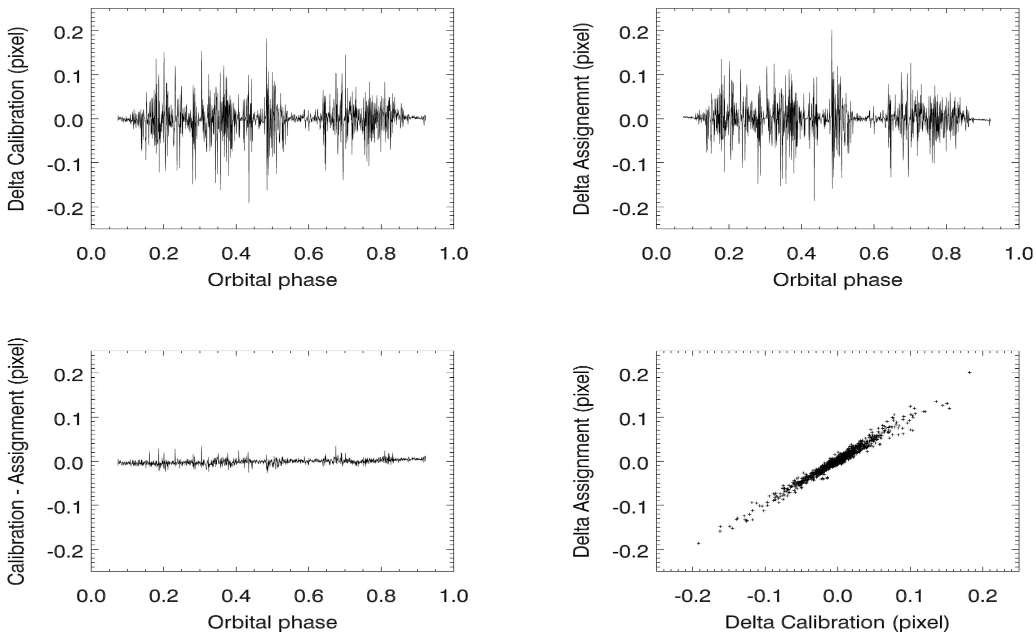

Fig.1 The top left panel shows the relative change in the first wavelength polynomial coefficient for a nadir pixel in the VIS channel, for orbit 3499 (12 March 2005), expressed in pixels. The top right shows the relative change in radiance multiplied by a pre-calculated factor. The bottom left panel shows the difference of the two top panels. The bottom right plots the observed shift (Delta Calibration) vs. the pre-calculated shift (Delta Assignment).

In order to be able to correct for the observed wavelength shifts, it is important that the derived conversion factors be stable in time. This turns out to be the case. This means that we can pre-calculate the conversion factors, based on a large number of orbits, in order to increase statistics and decrease noise, and apply those numbers to all observations. The orbit-to-orbit variability is on the order of 5 percent for the correction factors for the first wavelength polynomial. This variability is mainly statistical and largely reduced by averaging the correction factors of a large number of orbits, spread over a long period of time. The error in the derived correction of the wavelength scale due to the inhomogeneous slit illumination is in the order of 1 to 2 percent. So, for an initial shift of 0.1 pixel, the error made amounts to about $1/500^{th}$ to $1/1000^{th}$ of a pixel.

We also find that the amplitude of wavelength shift is dependent on the wavelength itself. That is, the effect that e.g. a passing cloud has on the spectral slit function is wavelength dependent. This is to be expected, because the slit function itself is wavelength dependent as well. Therefore, not only the first parameter in the wavelength parameterization needs to be modified, but higher order terms as well. This is also expressed by the fact that the relative change in the signal is not only strongly correlated with the first polynomial coefficient but with the second as well.

In the operational data processor, the polynomial coefficients that describe the wavelength (see equation 1) are modified:

$$c_i = c_i^{initial} + b_i \cdot \Delta Rad_{smp} \tag{3}$$

where $c_i^{initial}$ are the wavelength coefficients after the small temperature correction has been applied, b_i are the pre-calculated conversion coefficients. After that, the wavelengths are calculated using equation 1. This method was implemented in the data processing software in February 2005 and it is found to work as expected. A more detailed description of the in-flight wavelength calibration for OMI is given in [7].

3 A New High Resolution Solar Reference Spectrum

As will be clear from the previous paragraph, one of the most important ingredients for the wavelength calibration to work properly is a high resolution solar reference spectrum. We found that the available solar reference spectra ([6],[8],[9]) needed further improvement for use in the analysis of the OMI solar measurement data, in terms of spectral resolution or radiometric accuracy. This led us to construct a new high resolution solar reference spectrum. Broadly speaking we can divide the existing solar reference spectra in two groups, based on spectral resolution. We consider low resolution to be above

0.1 nm and high resolution below. This limit is determined by the spectral resolution and sampling of OMI spectra. The main use of the high resolution spectrum is by convolving it with OMI slit function, in order to obtain a spectrum at OMI resolution. For this, the spectral resolution of the input spectrum needs to be at least a factor of 5 higher than that of the resulting spectrum.

Only a few high resolution solar spectra in the UV-VIS domain are available. One for the most widely used spectra is that of Chance and Spurr [6]. This is a composite of the a high resolution UV-balloon spectrum, covering the wavelength range between 200 and 310 nm and ground based spectra obtained at Kitt Peak, covering the range between 296 and 1200 nm. The accuracy of the wavelength scale was estimated to be 0.002 nm below 300 nm and 0.001 nm above 305 nm. The combined spectrum is at 0.01 nm sampling and at 0.025 nm resolution. A high resolution solar reference spectrum based on an accurate model of the sun is [8]. A clear advantage of model spectra is the unlimited spectral coverage and resolution one can obtain. However, we found that the radiometric accuracy as well as the relative strength of many Fraunhofer lines in the spectrum insufficiently matched the observations.

The most widely used low resolution solar reference spectrum is that of Thuillier et al. (2003) [10]. This spectrum, with coverage between 200 and 2400 nm is also a composite spectrum, based on measurements with the satellite instruments SOLSPEC and SOSP. Most of their effort has gone into ensuring excellent radiometric accuracy. The precise spectral resolution of the spectrum is not quoted in the paper. The SOLSPEC data (between 200 and 850 nm) were measured at 1 nm resolution and the Fraunhofer lines from Kurucz and Bell were installed at 1 nm resolution. This suggests that the spectral resolution (between 200 and 850 nm) is 1 nm. Most comparisons of this spectrum with known reference spectra were performed at 5nm resolution.

3.1 Method

Here we describe the method that aims to combine the best properties of the above sun spectra, in order to construct a high resolution solar reference spectrum with sufficient radiometric accuracy. The method we used consists of four steps:

(1) Convolve a high resolution spectrum with less accurate radiometric calibration with the best slit function that is available for the lower-resolution solar reference spectrum: $F_{lores}^{hisamp} = F_{hires} \otimes S_{lores}$

(2) Interpolate the thus obtained high sampling, low-resolution spectrum on the wavelength grid of the low-resolution reference spectrum: $F_{lores}^{losamp} = \mathrm{Regrid}(F_{lores}^{hisamp})$

(3) Divide that spectrum by the low-res spectrum, to obtain the fraction by which to multiply the original high-resolution spectrum, used in 1: $Q^{losamp} = F_{lores}^{losamp} \big/ F_{lores}^{meas}$

(4) Interpolate the fraction from 3 to the high resolution wavelength grid: $Q^{hisamp} = \mathrm{Regrid}(Q^{losamp})$

The new high-resolution solar reference spectrum is then defined by: $F_{hires}^{REF} = Q^{hisamp} \cdot F_{hires}$

There are a number of issues that need to be considered in the above procedure:

- The original high resolution spectrum: in principle the spectrum from [4] can be used as a starting point. The merging of the UV and the VIS spectrum was improved.
- How to find the best low(er)-resolution reference spectrum: When using [10] in the above process the results we obtained were not optimal. Better results were obtained when using the high-resolution SUSIM spectra for wavelength less than 410 nm and a balloon spectrum [11] for longer wavelengths.
- How to determine the instrument transfer function (slit function) of the low-resolution instrument: in order to get the expected smooth multiplication factor Q^{losamp} we obtained the optimal slit functions for both the SUSIM and the balloon instruments.
- Interpolation between the low-resolution and the high-resolution spectra.

In order to show how much the high resolution solar reference spectrum has been improved as well as how well we understand the intricacies of the OMI instrument, in terms of spectral (a.o. slit function) and radiometric calibration, the ratio of an OMI measurement and the convolved high resolution solar reference spectrum is calculated. In Fig.2 we show the results for both the new and the old solar reference spectrum [5]. It can be observed that the new reference spectrum results in far less residual structure (top line) than the older sun reference spectrum (bottom line).

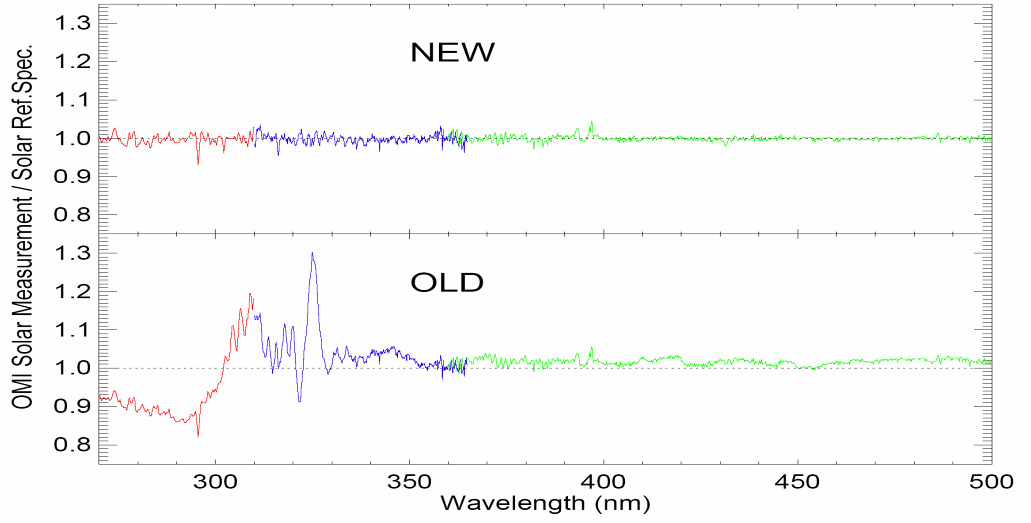

Fig.2 The top panel shows the fraction of an OMI solar measurement and the convolved high resolution solar reference spectrum. The bottom shows the same, but with the old solar reference spectrum.

4 Conclusions

In this paper we describe two subjects that concern the wavelength calibration of the Ozone Monitoring Instrument. The first concerns the unexpected in-flight variability of the wavelength scale of the radiance spectra. The wavelength scale can change by a few tenths of a pixel, whereas the required accuracy is $1/100^{th}$ of a pixel. This variability can be traced back to the optics of the instrument. By using higher frequency radiance data also available from the OMI L1B product, we can account for these variations and obtain the required accuracy of $1/100^{th}$ of a pixel. The above mechanism is not typical for OMI alone, but can also play an important role in other hyperspectral Earth observation spectrometers with comparable resolution and field-of-view size. However, scanning spectrometers like GOME and SCIAMACHY will suffer less from this mechanism since they scan a much larger ground scene.

The second issue addressed in this paper is the construction of a new high resolution solar reference spectrum. Such a spectrum is needed in the in-flight wavelength calibration process. The currently available spectra insufficiently matched our needs. It is shown that our updated version provides a much better agreement with the measured solar spectra by OMI.

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