

How big is an OMI pixel?

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1 Abstract.

2 The Ozone Monitoring Instrument (OMI) is a push-broom imaging spectrometer, observing solar
3 radiation backscattered by the Earth's atmosphere and surface. The incoming radiation is detected
4 using a static imaging CCD detector array with no moving parts, as opposed to most of the previous
5 satellite spectrometers, which used a moving mirror to scan the Earth in the across-track direction.
6 The sensitivity function of the Field of View (FoV) of detector pixels, projected on the Earth, is
7 defined as the point spread function (PSF). The OMI PSF is not quadrangular, which is common
8 for scanning instruments, but rather super-Gaussian shaped and overlapping with the PSF of neigh-
9 bouring pixels. This has consequences for pixel-area dependent applications, like e.g. cloud fraction
10 products, and visualisation.

11 The shape and sizes of OMI PSFs were determined pre-flight by theoretical and experimental tests,
12 but never verified after launch. In this paper the OMI PSF is characterised using collocated MODer-
13 ate resolution Imaging Spectroradiometer (MODIS) reflectance measurements. MODIS measure-
14 ments have a much higher spatial resolution than OMI measurements and spectrally overlap at
15 469 nm. The OMI PSF was verified by finding the highest correlation between MODIS and OMI re-
16 flectances in cloud-free scenes, assuming a 2D super-Gaussian function with varying size and shape
17 to represent the OMI PSF. Our results show that the OMPIXCOR product 75FoV corner coordinates
18 are accurate as the Full Width at Half Maximum (FWHM) of a super-Gaussian PSF model, when this
19 function is assumed. The softness of the function edges, modelled by the super-Gaussian exponents,
20 is different in both directions, and view angle dependent.

21 The optimal overlap function between OMI and MODIS reflectances is scene dependent, and
22 highly dependent on time differences between overpasses, especially with clouds in the scene. For
23 partially clouded scenes, the optimal overlap function was represented by super-Gaussian exponents
24 around 1 or smaller, which indicates that this function is unsuitable to represent the overlap sensitiv-
25 ity function in these cases. This was especially true for scenes before 2008, when the time differences
26 between Aqua and Aura overpasses was about 15 minutes, instead of 8 minutes after 2008. During
27 the time between overpasses, clouds change the scene reflectance, reducing the correlation and in-
28 fluencing the shape of the optimal overlap function.

29 1 Introduction

30 The Ozone Monitoring Instrument (OMI) (Levelt et al., 2006) was launched in 2004 on-board the
31 Aura satellite, in a polar, sun-synchronous orbit at approximately 705 km altitude, with a local equa-
32 torial crossing-time of 13:45 (ascending node). Its main objective is to monitor trace gases in the
33 Earth atmosphere, especially ozone. It was built as the successor to the ESA instruments GOME
34 (Burrows et al., 1999) and SCIAMACHY (Bovensmann et al., 1999), and NASA's TOMS instru-
35 ments (e.g. Fleig et al., 1986; Bhartia et al., 2013). GOME and SCIAMACHY were the first space-
36 borne hyperspectral instruments, measuring the complete spectrum from the ultraviolet (UV) to
37 shortwave-infrared (SWIR) wavelength range with a relatively high spectral resolution (typically
38 0.2–1.5 nm), from which multiple trace gases, clouds and aerosol parameters can be retrieved simul-
39 taneously. TOMS instruments have been monitoring the ozone column at a relatively high spatial
40 resolution ($50 \times 50 \text{ km}^2$) with daily global coverage since 1978. OMI was designed to combine those
41 functions and measure the complete spectrum from the UV to the visible wavelength range (up to
42 500 nm) with a high spatial resolution and daily global coverage. To this end, the imaging optics
43 were completely redesigned.

44 Instead of a rotating mirror, in OMI a two-dimensional CCD detector array (780×576 pixels) is
45 used to map the incoming radiation in the across-track and wavelength dimensions simultaneously. A
46 swath of about 2600 km in the across-track direction is imaged along one dimension of the detector
47 array. Spectrally, the radiation is split into two UV channels and a visible (VIS) channel and imaged
48 along the wavelength dimension of the detector array. The spectral resolution of the VIS channel
49 is 0.63 nm. The along-track direction is scanned due to the movement of the satellite. In default
50 'Global' operation mode, five consecutive CCD images, each with a nominal exposure time of 0.4 s,
51 are electronically co-added during a two second interval. The sub-satellite point moves about 13 km
52 during this time interval (Levelt, 2002). The consequence of this design is that the spatial response
53 function of the OMI footprints is not box-shaped, but has a peak at the centre of the footprint. This
54 new design, avoiding moving parts, was used in OMI for the first time, and is now being used in
55 several new upcoming satellite missions.

56 The telescope Field of View (FoV) is determined by the projection of the OMI spectrograph
57 slit on the Earth's surface from the point of view of a CCD pixel. This projection is affected by
58 Fraunhofer diffraction of the imaging optics, which, for a circular aperture, can be modelled using an
59 Airy function. For a rectangular slit, used in OMI, the solution can be approximated by a Gaussian
60 function in two dimensions. The FoV has been determined pre-flight by measuring the intensity
61 response to a star stimulus for all pixels. The response function was measured by exposing the pixels
62 to a point source and rotating the instrument. The sensitivity curve found in this way was fitted
63 to a Gaussian curve, of which the Full Width at Half Maximum (FWHM) was reported. This is
64 proprietary information, but the results are summarised here. In the swath (across-track) direction
65 the average peak position for each pixel was determined and fitted to a linear curve to determine the

66 spatial sampling distance for the three channels, which gives the instantaneous FoVs in the across-
67 track direction for individual pixels. For the VIS channel the FoV for the entire swath is 115.1° . The
68 point spread function (PSF) in the across-track direction was not determined (or reported). However,
69 a memo from the OMI Science Support Team from 2005 shows an across-track pixel size estimation
70 from these measurements, where the sizes have been determined by assuming no overlap between
71 adjacent pixels and computing the distances between the peak positions when imaged on the earth.
72 This yields sizes in the across-track direction of 23.5 km at nadir and 126 km for far off-nadir (56
73 degrees) pixels.

74 In the along-track direction the FoV was characterised by tilting the instrument to simulate the
75 movement in the flight direction. The measurements were fitted to a Gaussian curve with variable
76 width for different across-track angles and wavelengths. This width is reported as the FWHM in
77 degrees, which is about 0.95 at nadir and 1.60 at 56 degrees for the VIS channel. This corresponds
78 to a nadir pixel size in the along-track direction of about 15 km and a far off-nadir pixel size of about
79 42 km, when the Gaussian is convolved with a boxcar function whose width is the 13 km movement
80 of the subsatellite point during the 2 second exposure.

81 The instantaneous FoV (iFoV) of the OMI instrument is influenced by a polarisation scrambler,
82 that transforms the incoming radiation from one polarisation state into a continuum of polarisation
83 states (as opposed to unpolarised light). The incoming beam is split into four beams of equal inten-
84 sity, scrambled, and projected onto the CCD. Since the projections of the four beams are slightly
85 shifted with respect to each other, the polarisation state of the incoming radiation still slightly deter-
86 mines the intensity distribution of the four beams and therefore the iFoV in the flight direction. The
87 only property which is not dependent on the polarisation state of the incoming radiation is the centre
88 of weight of the four beams. This corresponds to the centre of the ground pixels, which is therefore
89 the only geolocation coordinate that can be determined unambiguously (van den Oord, 2006).

90 Therefore, centre coordinates are provided in the Level 1b data product, but corner coordinates are
91 not. However, for mapping purposes, ground pixel area computations (e.g. for emission estimates per
92 unit area) and collocation, an OMI corner coordinate product was developed, called OMPIXCOR,
93 which is provided online via the OMI data portal (Kurosu and Celarier, 2010). Two sets of quadran-
94 gular corner coordinates are provided. One set contains *tiled* pixel coordinates, which are essentially
95 the midpoints between adjacent centre coordinates, mainly useful for visualisation purposes, as no
96 overlap between pixels is imposed. The other set contains so-called 75FoV pixel coordinates, which,
97 according to Kurosu and Celarier (2010), correspond to 75% of the energy in the along-track FoV.
98 The authors assumed a 1° FWHM for the iFoV to fix a Gaussian distribution and convolved it with
99 a boxcar to model the satellite movement. The area under a Gaussian curve corresponds to about
100 76% at FWHM for a normal distribution (exponent of 2), however, the authors claim to have used a
101 super-Gaussian with exponent of 4 for this. In this case the energy contained within the FWHM has
102 increased to about 89%. When this iFoV is convolved with the boxcar function, the energy within

the FWHM will have increased even more. The 75FoV pixels generally overlap in the along-track direction, since radiation emanating from successive scans enter the FoV. The coordinates in the across-track direction, however, are still the half-way points between adjacent pixels.

The application of quadrangular pixel shapes for OMI can become problematic when pixel values are aggregated onto a regular grid (e.g. Level 3 products that are reported on a regular lat-lon grid). If pixels overlap, which might occur when several orbits are averaged or in case of 75FoV pixels, extreme values may be smoothed and reduced due to averaging. A more realistic distribution that preserves mean values can be reconstructed using a parabolic spline surface on the quadrangular grid, resulting in a much better visualisation (Kuhlmann et al., 2014). In cases where values from OMI are compared with that of another instrument, especially with a higher spatial resolution, the approximate true shape of an OMI pixel is desired. For example, we intend to combine spectral measurements from OMI and MODIS to determine the aerosol direct effect over clouds (de Graaf et al., 2012). To this end, an optimal characterisation of the PSF of the OMI footprint is desired, to optimise the accuracy of the retrieval.

In this paper, the OMI PSF for the VIS channel is investigated by testing various predefined shapes and sizes under various circumstances and determining the maximal correlation between OMI and MODIS reflectances. In section 2, the consistency between overlapping OMI and MODIS reflectances is investigated. A cloud-free scene from 2008 is used to study the PSF under the most optimal circumstances. In chapter 3, a two dimensional super-Gaussian function with a varying exponent is introduced, which can change shape from a near-quadrangular to a sharp-peaked distribution. Furthermore, the sizes in both along and across-track directions can be varied. This function is used to define various PSFs, which are investigated for various scenes. The change in PSF is further investigated by looking into the effect of scene and geometry changes during the (varying) overpass times of OMI and MODIS. The conclusions from this study are reported in section 4. The geolocations of the pixels in the UV channels are slightly different from those in the VIS channel. However, the PSF cannot be determined in the same way for the UV, since MODIS measurements do not overlap with these channels spectrally.

2 Data

The Aura satellite flies in formation with the Aqua satellite in the Afternoon constellation (A-train). Aqua was launched in 2002, to lead Aura in the A-train by about 15 minutes. The time difference between the instruments within the A-train is controlled by keeping the various satellites within control-boxes, which are defined as the maximum distances to which the satellites are allowed to drift before correcting manoeuvres are executed. Therefore, the time difference between OMI and MODIS is variable by up to a few minutes. A major orbital manoeuvre in 2008 of Aqua decreased the distance between the Aura and Aqua control boxes to about 8 minutes.

138 To investigate the correlation between OMI and MODIS observed reflectances, several scenes
139 were selected. One reference scene will be discussed here in detail. It was an almost cloud-free
140 scene over the Sahara desert on 4 November 2008, around 14:00 UTC (start of the first MODIS
141 granule). At this point in time, the time difference between OMI and MODIS was reduced to 8
142 minutes and around 20 – 30 seconds, depending on the pixel row. The differences between the pixel
143 times arise from the fact that MODIS has a scanning mirror, while OMI has no scanning optics, but
144 exposes the CCD to different scenes while moving in the flight direction. The scene is visualised
145 in Figure 1, using MODIS channels 2, 1, and 3 to create an RGB picture at 1 km² resolution. The
146 MODIS granules are outlined in yellow, while the considered OMI scene is outlined in red. From
147 June 2007 onward, OMI suffered from a degradation of the observed signal in an increasing number
148 of rows, called the row anomaly (OMI row anomaly team, 2012). In November 2008 the anomaly
149 was limited to only rows 53 and 54 for scenes near the equator. These rows were disregarded in the
150 comparison. In order to stay within the MODIS swath the OMI swath was further reduced to rows 2
151 to 57. A total of 7,335 OMI pixels are left in the scene.

152 To compare reflectances from OMI and MODIS, the reflectance measured by OMI is convolved
153 with the MODIS spectral response function. MODIS channel 3 at 469 nm overlaps with the OMI
154 VIS channel (350 – 500 nm). This is illustrated in Figure 2, where two OMI reflectance spectra from
155 the VIS channel are plotted, together with the normalised MODIS response function of channel 3
156 (red curve). The reflectance spectra correspond to the darkest and brightest pixels (at 469 nm) in
157 Figure 1, indicated by the green boxes. The darkest pixel is a vegetated area with an OMI reflectance
158 of 0.0935 and the brightest pixel is a cloud covered scene with an OMI reflectance of 0.5040, both
159 at 469 nm.

160 All the 7,335 OMI pixels in the scene in Figure 1 were compared to collocated MODIS pixels, see
161 the left panel of Figure 3. Here, all the MODIS pixels that fall (partly) within an OMI quadrangular
162 pixel, as defined by the OMPIXCOR 75FoV corner coordinates, are averaged with equal weight,
163 which is the easiest and quickest averaging strategy. The MODIS reflectances are somewhat lower
164 than the OMI reflectances; a linear fit through the points shows a slope of 0.959 and an offset of
165 0.0023. The MODIS reflectances show a Pearson's correlation coefficient r of 0.998 with the OMI
166 reflectances, and a standard deviation (SD) of 0.0039. The SD refers to the RMS deviation of the
167 measurements to the model fit.

168 3 OMI point spread function

169 The true PSF of an OMI pixel is expected to resemble a flat-top Gaussian shape. To investigate the
170 OMI PSF, the response at 469 nm is compared to the MODIS channel 3 signals, weighted using
171 different super-Gaussian functions in two dimensions, and checking the change in the correlation

172 and SD between the OMI and MODIS reflectances. A 2D super-Gaussian distribution is defined by

$$173 \quad g(x, y) = \exp \left(-\left(\frac{x}{w_x}\right)^n - \left(\frac{y}{w_y}\right)^m \right), \quad (1)$$

174 where x and y are the along and across-track directions, and $w_{x,y}$ are the weights in either direction,
175 defined by

$$176 \quad w_x = \frac{\text{FWHM}_x}{2(\log 2)^{1/n}}; \quad w_y = \frac{\text{FWHM}_y}{2(\log 2)^{1/m}}. \quad (2)$$

177 $\text{FWHM}_{x,y}$ are the full widths at half maximum in the along and across-track directions, respectively,
178 defined in this paper by the 75FoV pixel corner coordinates. The size of the PSF model can be varied
179 to include more or fewer MODIS pixels from neighbouring pixels in the along and across-track
180 directions by varying w_x and w_y . All size changes are reported relative to FWHM_x and FWHM_y .

181 The shape of the PSF model is determined by the Gaussian exponents n and m , which define
182 the ‘pointedness’ of the distribution. In one dimension, $n = 2$ corresponds to a normal distribution,
183 $n < 2$ results in a point-hat distribution and $n > 2$ results in a flat-top distribution, see the illustration
184 in Figure 4. Various PSF models are illustrated in Figure 5. The colours of the square MODIS pixels
185 indicate the relative contribution of that pixel. The different panels show OMI pixels at different
186 rows, to illustrate the change in orientation and number of MODIS pixels that fall inside an OMI
187 pixel when the viewing zenith angle changes. Figure 5a shows the quadrangular OMI pixel, with
188 all MODIS pixels within the OMI corner coordinates having equal weight, while all pixels outside
189 the footprint have zero weight. Figure 5b shows a 2D flat-top super-Gaussian ($n = m = 8$) shape
190 using the 75FoV corner coordinates to constrain the FWHM, resembling the quadrangular shape
191 but with smoother edges. Figure 5c shows a 2D super-Gaussian distribution, with $n = 2, m = 4$,
192 which represents the optimal representation of the PSF using a super-Gaussian function. Figure 5d
193 shows a 2D point-hat super-Gaussian ($n = 1, m = 1.5$) distribution, which is the optimal fit of this
194 function when broken clouds are in the scene. Figures 5e and f show the weights for pixels which are
195 assumed to be twice as wide or long as the 75FoV pixels and using a 2D super-Gaussian distribution
196 with $n = 2, m = 4$.

197 The size and shape of the PSF model was varied by changing n from 0.5 to 16, m from 1 to 16,
198 and the FWHM from 0.5 to 3 times the 75FoV corner coordinates. For each configuration the corre-
199 lation between the OMI and MODIS reflectances and the SD were determined, using all pixels from
200 the scene in Figure 1. The correlation change is shown in Figure 6. The blue dashed-dotted curve
201 shows the change in correlation for a changing Gaussian exponent and 1·FWHM, i.e. the change
202 in PSF model shape and 75FoV corner coordinates to constrain the FWHM. In the top panel the
203 change in correlation coefficient r is shown for a changing Gaussian exponent n using the optimal
204 Gaussian exponent found for the across-track direction $m = 4$. For this function the optimal Gaus-
205 sian exponent in the along-track direction is $n = 2$. The blue dotted curve shows the goodness-of-fit
206 q corresponding to each of the correlation coefficients r (the blue dashed-dotted line). It was deter-
207 mined using a constant error for OMI measurements, and a constant error for MODIS measurements

but weighted by the number of MODIS pixels in each OMI pixel. It shows a reasonably good fit at the optimum $n = 2$.

The red line shows the change in correlation when the along-track width is varied. The shown curve is for the optimal Gaussian parameters, $n = 2, m = 4$, and peaks at 1.0, meaning that the 75FoV corner coordinates are the optimal sizes to constrain the FWHM when a super-Gaussian model is used. The lower panel shows the same dependencies in the across-track direction. The change of r for changing m (the shown dashed-dotted line is for the optimal Gaussian exponent $n = 2$) and the red curve is the width in the across-track direction for $n = 2, m = 4$. The red curve also peaks at one, again confirming the 75FoV corner coordinates, while m peaks at 4. However, the change for larger m is minimal, meaning that the softness of the edges in the across-track direction make very little difference. Only the goodness-of-fit q decreases significantly for larger m , so $m = 4$ can be used as the optimal parameter. These four optimal parameters are also the absolute maximum in the entire parameter space, with $r = 0.998$. This is noticeably higher than the correlation when quadrangular pixels are used.

The correlation between the OMI and MODIS reflectances and the SD, when the optimal PSF model for this scene is used, is shown in the right panel of Figure 3. The SD for the optimal PSF is 0.0036. The change in SD for different shapes and sizes is not shown, because it is consistent with the change of the reciprocal of the correlation, in the sense that it is minimal when the correlation peaks and can be equally used to find the optimal PSF characterisation in this way.

3.1 PSF sensitivity

When a super-Gaussian form is assumed, the optimal super-Gaussian model parameters for the reference scene are $n = 2, m = 4$ and the 75FoV corner coordinates for the Gaussian FWHM. However, the correlation between OMI and MODIS reflectances is not a constant. A number of scenes were investigated to show the change in correlation between OMI and MODIS reflectances in time and space.

First, another cloud-free scene was found over the Middle East on 7 October 2008, starting on 10:20 UTC, see Figure 7. The time difference between OMI and MODIS is about 8 minutes and 34–45 s. This scene is entirely cloud-free over land, and the reflectance ranges from 0.12 over the ocean to 0.41 over the desert. The correlation between the OMI and MODIS reflectances is depicted in the right panel of Figure 7, which displays the same dependencies as in Figure 6. The highest correlation ($r = 0.9977$) was found for the same super-Gaussian parameters as before, confirming the optimal OMI PSF model. Only the goodness-of-fit was slightly lower than before, indicating a lower correlation between the OMI and MODIS reflectances.

241 3.2 Viewing angle dependence

242 Next, a scene over Australia was selected on 11 October 2008 starting on 04:45 UTC, see Figure 8.
243 The time difference between OMI and MODIS is about 8 minutes and 35–43 s. This scene has a
244 large cloud-free part, but also a large cloudy part. Most cloud pixels, indicated by the red rectangles,
245 were not used in the analysis. The correlation between OMI and MODIS for various shapes and
246 sizes is again displayed in the right panel. The maximum correlation for this scene was lower than
247 before, $r = 0.9927$, and obtained for a point-hat super-Gaussian distribution with exponents $n = 1.5$
248 and $m = 2$, and FWHM corner coordinates. The goodness-of-fit is significantly lower than before.

249 One reason for the lower Gaussian exponents of the 2008 Australian scene in the across-track
250 direction is the removal of the pixels at the end of the swath, which were filtered because of the
251 clouds in those pixels. The OMI PSF is dependent on the pixel row, or viewing angle, with wider
252 PSFs at the swath ends. Since most of the cloud pixels are at the swath ends, removing these pixels
253 removes the larger exponents. The viewing angle dependence of the PSF is treated here.

254 Since the OMI FoV is dependent on the polarisation of the scene, the PSF should also be de-
255 pendent on the scattering geometry. Furthermore, the diffraction at the edges of the FoV can be
256 distinctly different for FoVs at nadir compared to those with a large viewing zenith angle (VZA). To
257 investigate this effect, the OMI PSF was characterised using a super-Gaussian function dependent on
258 VZA. For all the scenes described in this paper, the optimal super-Gaussian shape was determined
259 per OMI pixel row, by varying the Gaussian exponent and determining the maximum correlation
260 between OMI and MODIS pixels for each pixel row. Then the optimal exponents were averaged
261 and plotted as a function of pixel row. In this analysis, the 75FoV pixel sizes were used, to reduce
262 the number of variables and because the above analysis showed that the 75FoV corner coordinates
263 are good indicators of the pixel sizes for Gaussian shapes. The result is shown in Figure 9. The
264 super-Gaussian exponents are rather wildly fluctuating, because they have a limited sensitivity near
265 the optimum, especially m . Averaging over the scenes reduces this, but is somewhat arbitrary. In
266 Figure 9 a boxcar average over 5 neighbouring points is shown as well.

267 Still, some change in Gaussian exponents can be observed as a function of VZA. The Gaussian
268 exponent in the across-track direction m changes from around 3–4 at nadir to about 7 at far off-nadir.
269 Also n is VZA dependent, changing from about 1.5 at nadir to more than 2 at the swath edges. The
270 reason for the increasing exponents towards the swath edges is the pixel size increase towards the
271 swath edges. The pixel sizes are shown for reference. FoVs at larger VZA are much wider, changing
272 the optimal super-Gaussian that fit the PSF. Furthermore, as observed before, the diffraction at the
273 edges of the FoV will be different at larger viewing angle.

274 3.3 Scene dependencies

275 The smaller Gaussian exponents for the 2008 Australian scene (Figure 8) are only partly explained
276 by the VZA dependence. The Gaussian exponent $n < 2$ indicates a point-hat super-Gaussian distri-
277 bution in the along-track direction, which is, as Figure 5e shows, a distribution that is physically
278 unlikely. For this scene, the super-Gaussian function is apparently not a good representation of the
279 PSF of the OMI FoV. The reason for this mismatch are broken cloud fields in the scene, which
280 change the scene reflectance between overpasses of Aqua and Aura. Scene dependencies will be
281 investigated below.

282 The overpass time between Aqua and Aura changed in 2008, when a correcting manoeuvre
283 brought OMI closer to MODIS. To illustrate the effect, another Sahara cloud-free scene in the begin-
284 ning of 2008 was selected, when the manoeuvre had not yet been performed, see Figure 10. The time
285 difference between the instruments for this scene is as large as around 14 minutes, up to 16 minutes
286 and 26 s. In this case, the highest correlation is found for a super-Gaussian distribution with expo-
287 nents $n = 1.5$, $m = 2$, which is again a point-hat super-Gaussian distribution. Similarly, when the
288 shape is fixed to the optimal Gaussian exponents, the highest correlation is found for pixel sizes
289 that are wider than the 75FoV corner coordinates, see the red curves in Figure 10. This is different
290 from the reference scene in Figure 1. The maximum correlation for this scene is $r = 0.982$, which is
291 lower than for the reference scene, in December 2008. The goodness-of-fit q shows much lower val-
292 ues, showing the difficulty with the used PSF model to correlate the OMI and MODIS reflectances.
293 Apparently, the time difference between the Aqua and Aura of 15 minutes makes a comparison be-
294 tween the two instruments much more challenging, even for almost cloud-free scenes. It is unlikely
295 that the OMI FoV has changed much between January and December 2008. Furthermore, a cloud-
296 free Sahara scene in 2006 (31 January 2006, around 13:55 UTC, not shown), showed the same lower
297 correlation, peaking for the same Gaussian exponents.

298 The effect of changing scenes between overpasses can be illustrated by looking at the pixels with
299 the highest SD between the OMI reflectances and the average collocated MODIS reflectances. Even
300 for a scene after 2008, when the overpass time difference is reduced to about 8 minutes, the retrieved
301 TOA reflectance can change significantly during this time in the case of broken clouds. The pixels
302 with the highest SD for the reference scene were marked blue in the right panel of Figure 3. The
303 marked points correspond to the blue coloured OMI pixels in Figure 1, which are the areas where
304 the scene contains broken cloud fields. In the few minutes between Aqua and Aura overpasses these
305 clouds change shape and position, changing the average reflectance in a pixel when the cloud fraction
306 is changed.

307 This is the main reason for the small optimal super-Gaussian exponent for the 2008 Sahara scene
308 (Figure 10) and the Australian scene (Figure 8): due to scene changes during the different overpass
309 times, the observed overlap function deviates from the true PSF, which closely resembles a Gaus-
310 sian or flat-topped Gaussian. Instead a more point-hat distribution with wider wings is found. The

311 centre coordinates have the relative highest correlation, but lower than before, while the correlation
312 becomes smoothed over a larger area, giving the tails of the function a higher correlation than for
313 the true PSF.

314 3.4 Accuracy of combining OMI and MODIS

315 The optimal overlap function for MODIS pixels within an OMI FoV can now be determined for
316 practical purposes, i.e. mixed scenes with ocean, land and clouds. This is needed to determine the
317 accuracy that can be expected when OMI and MODIS measurements are combined to reconstruct the
318 reflectance spectrum for the entire shortwave spectrum. To determine the accuracy, the correlation
319 between collocated OMI and MODIS reflectances and the SD was determined by comparing the
320 instruments for the scene shown in Figure 11. This scene was taken on 13 June 2006, starting on
321 13:33 UTC when the time difference between the instruments was about 15 minutes. The scene
322 contains a mixture of land and ocean scenes, with and without clouds, and also smoke from biomass
323 burning on the African continent. Only OMI rows 10–50 were processed, which will often be the
324 case to avoid problems with large pixels or extreme viewing angles. The optimal correlation was
325 found for super-Gaussian exponents $n = 1, m = 1.5$ and 75FoV corner coordinates (not shown).
326 The low Gaussian exponents can again be explained from the presence of clouds that change the
327 scene between the overpasses, and the exclusion of wide pixels at the swath edges. The correlation
328 between the OMI and MODIS reflectances using this shape is shown in the right panel of Figure 11.
329 Obviously, the correlation is a lot lower than for cloud-free scenes ($r = 0.964$). The SD is 0.0371,
330 which must be taken into account when OMI and MODIS reflectances are compared or combined.
331 Furthermore, the slope of a linear fit between the OMI and MODIS reflectance is 0.941, which is
332 smaller than that for cloud-free scenes, which showed about 4% difference. This larger range in
333 reflectances for cloud scenes apparently off-sets the difference between the instruments even further.

334 3.5 Geometry differences

335 The 4-5% difference between OMI and aggregated MODIS reflectances at 469 nm (Figure 3) can be
336 governed by changes in viewing and solar conditions between OMI and MODIS. Since the optics
337 and sub-satellite points differ for both instruments, the viewing angles are slightly different, even if
338 the satellites roughly follow the same orbit. More importantly, since Aura is always behind Aqua,
339 the solar zenith angle for OMI is always different from that of MODIS.

340 To investigate the effect of the differences in scattering geometry on the measured TOA re-
341 flectance, a cloud-free Rayleigh reflectance was modelled for each OMI pixel in the reference scene
342 in Figure 1. Each pixel was simulated twice, once using the OMI scattering geometry and once using
343 an average MODIS scattering geometry. In this way the expected reflectance difference can be de-
344 termined due to the difference in overpass time, keeping all else the same. To determine the average
345 MODIS reflectance, the simulated radiances were averaged over the OMI footprint using the opti-

mal flat-top Gaussian distribution with $n = 2, m = 4$, as was determined for this scene (Figure 6). The average radiance was then divided by the cosine of the solar zenith angle of the MODIS pixel which is closest to the centre of the OMI pixel. In this way, the most representative solar zenith angle is used to normalise the radiances. A realistic surface albedo was taken for each pixel, in order to make the model results comparable to the observations. The surface albedo database used was the TERRA/MODIS spatially completed snow-free diffuse bihemispherical land surface albedo database (Moody et al., 2005). The monochromatic calculations were performed at 469 nm, using a standard Rayleigh atmosphere (Anderson et al., 1986) reaching to sea level, and an ozone column of 334 DU. The results are shown in Figure 12.

The reflectance ranges from about 0.085 to 0.28, depending on the surface albedo, which is smaller than the observed reflectances (cf. Figure 3, right panel). This is mainly due to the clouds in the scene which are not simulated. The simulated OMI reflectances are larger than the simulated MODIS reflectances due to different geometries, like the observations. There is a small dependence on VZA, as shown in the right panel of Figure 12, where the relative differences between the OMI and MODIS reflectances are plotted as a function of either reflectance, to highlight the change for changing VZA (in colours). However, the difference between the simulated OMI and MODIS reflectances, with a slope of 0.9965 and an offset of -0.001 , is much smaller than between the observations. Therefore, we conclude that geometry differences between OMI and MODIS introduce differences of less than 1% and cannot explain the observed slope between OMI and MODIS reflectances. Most likely, calibration differences are causing the difference between the observed reflectances. The simulated correlation and SD are also notably better than for the observed scene. As noted before, clouds have the largest impact on the correlation between the observed reflectances of a scene.

4 Conclusions

The correlation between OMI and collocated MODIS reflectances was determined, to intercompare the performance of the instruments and to find the PSF of the OMI footprint. MODIS channel 3 at 469 nm overlaps with OMI's visible channel, and the signals can be compared when the reflectance signal of OMI is multiplied with the MODIS spectral response function, and MODIS reflectances are aggregated over the OMI footprint.

Due to the design of the OMI CCD detector array and the optical path, the footprint of OMI is not quadrangular and light from successive scans enters the OMI FoV. The shape and size of the PSF of the FoV was determined for a cloud-free scene, to eliminate, as much as possible, scene changes due to the different overpass times of Aura and Aqua. Assuming a super-Gaussian shape with variable exponents and FWHM, the best characterisation of the OMI PSF was found for an exponent $n = 2, m = 4$ and 1×75 FoV corner coordinates to constrain the FWHM.

380 The OMI PSF changes as a function of viewing angle. When the FWHM are fixed, the Gaussian
381 exponent ranges from about 1.5 at nadir to more than 2 at the swath edges, while m ranges from about
382 3-7. This is mainly due to the increase in pixel size for off-nadir angles. Furthermore, the diffraction
383 at the FoV edges is viewing angle dependent, and the OMI PSF is dependent on polarisation, due to
384 the presence of a polarisation scrambler in the OMI optical path.

385 The OMI-MODIS overlap function is scene dependent. In particular, for larger time differences
386 between the Aqua and Aura overpasses, the optimal overlap function shape is found for smaller
387 Gaussian exponents and wider overlaps. When the scene changes between overpasses the signal is
388 spread over a larger area, centred around the centre coordinate. Therefore, a more optimal overlap
389 function is found for a point-hat distribution with wider wings. This is especially true for cloud
390 scenes, which are most frequent. The correlation decreases, and the SD increases when clouds are in
391 the scene, and this can be used as an indication of the expected accuracy of a comparison between
392 OMI and MODIS reflectances. For a scene with broken clouds over both land and ocean in 2006,
393 an optimal Gaussian exponent of $n = 1, m = 1.5$ was found. In general, the changes in correlation
394 coefficient are small for small changes of the Gaussian exponents (much smaller than e.g. changes
395 due to time differences). The true OMI PSF is approximated by a super-Gaussian distribution with
396 exponent $n = 2, m = 4$ and 75FoV corner coordinates.

397 The use of non-scanning optics like those of OMI will be continued in new instruments, in par-
398 ticular TropOMI/Sentinel-5P (Veefkind et al., 2012), to be launched in 2016. For TropOMI, a cloud
399 masking feature is anticipated from Suomi-NPP/VIIRS (Schueler et al., 2002). Sentinel-5P will fly
400 in ‘loose formation’ with Suomi-NPP, with expected overpass time differences of about 5 minutes.
401 The results from this study are relevant for that mission, since such an overpass time difference will
402 significantly change the overlap function between TropOMI and VIIRS, and affect the accuracy of a
403 cloud mask from VIIRS. High resolution VIIRS measurements can be used in the way presented in
404 this paper to study and characterise the TropOMI PSF and the accuracy of the cloud mask.

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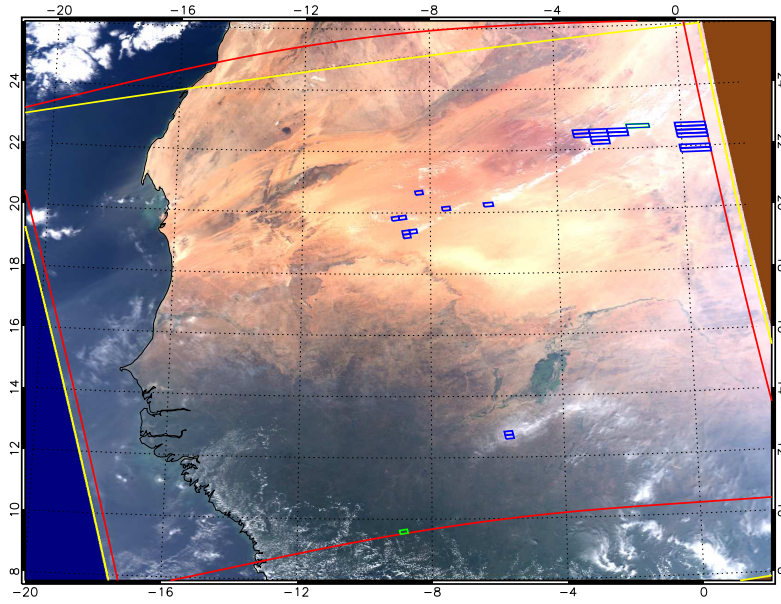


Figure 1. MODIS RGB image of the reference scene on 4 November 2008, 14:00 UTC (start of the central MODIS granule). The yellow lines indicate the MODIS data granules and the red lines the considered OMI swath, which was confined to rows 2–57, with the exception of pixels in the row anomaly (see text). The green pixels indicate the darkest (vegetated) and the brightest (cloud covered) areas in the scene. The OMI reflectance spectra of these pixels are shown in Figure 2. The blue OMI pixels correspond to the blue marked points in Figure 3.

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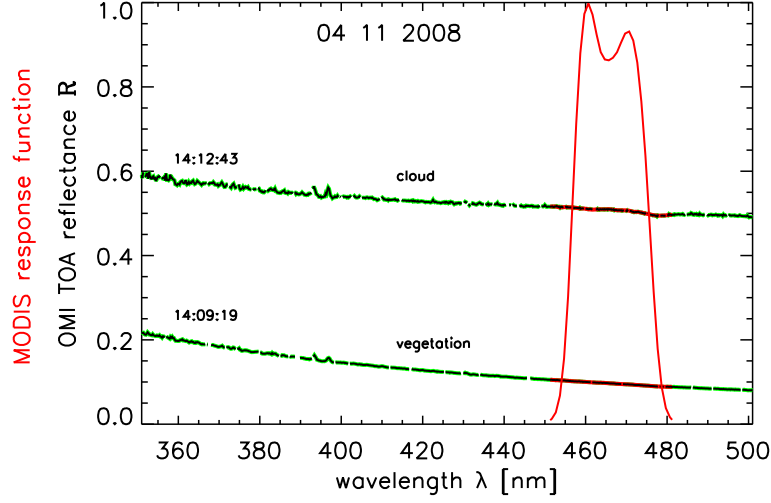


Figure 2. OMI top-of-atmosphere reflectance spectra on 4 November 2008, 13:37:24 UTC, and 13:38:02 UTC, of the green pixels in Figure 1 (black/green); and the normalised MODIS response function of channel 3 (red).

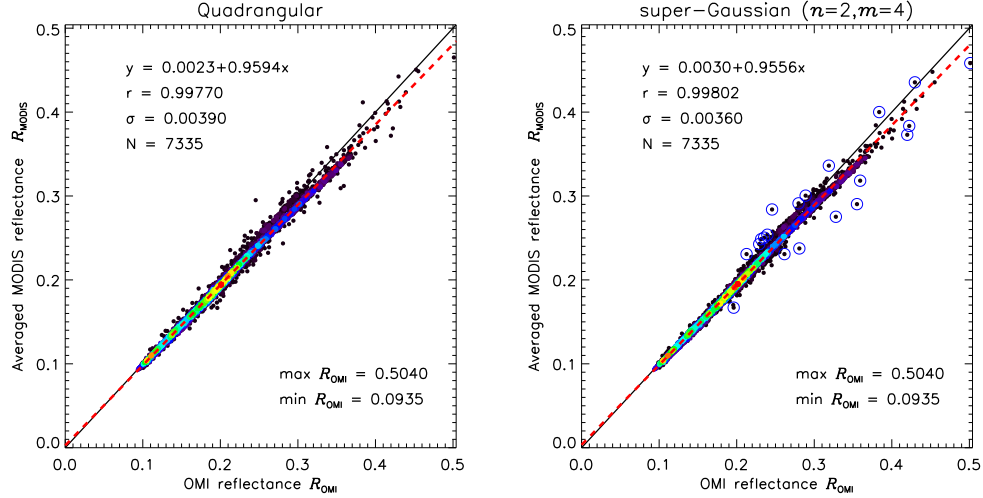


Figure 3. Scatter plot of OMI and MODIS collocated reflectances for the scene in Figure 1 using quadrangular OMI pixels (left panel) and optimised super-Gaussian ($n=2, m=4$) pixels (right panel). The red dashed line is the linear least squares fit to the measurements, given by the linear function $y = a_0 + a_1x$ in the plot. r is Pearson's correlation coefficient and σ the standard deviation of the points to the fitted line. The blue marked points have the largest σ and correspond to the blue OMI pixels in Figure 1. N is the number of points and $\max R_{\text{OMI}}$ and $\min R_{\text{OMI}}$ the maximum and minimum value in the plot, respectively.

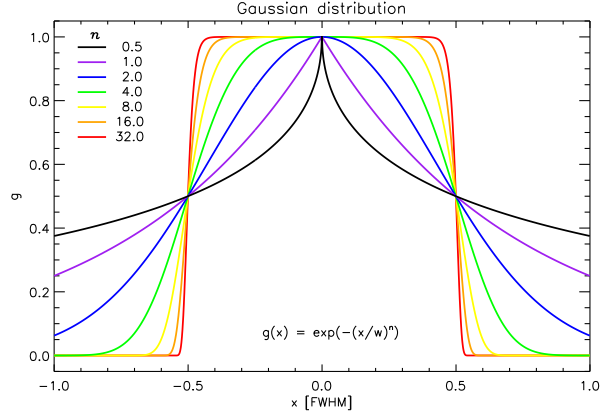


Figure 4. One dimensional normalised super-Gaussian distribution functions with varying exponents n . The normal distribution ($n = 2$) is plotted in blue.

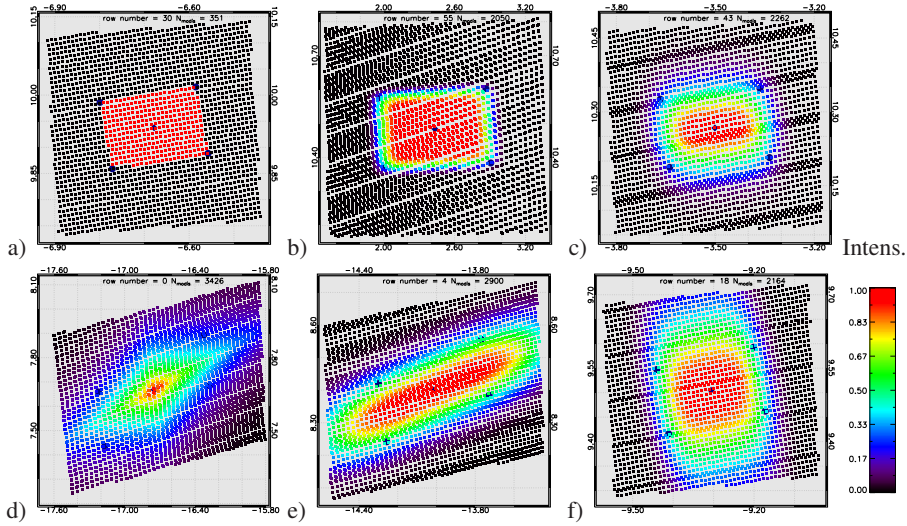


Figure 5. OMI 75FoV corner coordinates (dark blue filled circles), with the OMI centre coordinate (dark blue diamond), and collocated MODIS centre coordinates (black and coloured squares). The colours of the squares indicate the weighting of the MODIS pixels as indicated by the colour bar. a) Quadrangular weighting, with all MODIS pixels within the corner coordinates having equal weights, everything else disregarded; b) a 2D flat-top super-Gaussian with exponents $n = m = 8$, resembling the quadrangular shape with smoothed edges; c) a 2D super-Gaussian distribution with $n = 2$ and $m = 4$; d) a 2D point-hat super-Gaussian distribution with exponents $n = 1, m = 2$; e) a 2D super-Gaussian distribution ($n = 2, m = 4$) with twice the width in the across-track direction; f) a 2D super-Gaussian distribution ($n = 2, m = 4$) with twice the width in the along-track direction. Different OMI row number are shown (see panel captions) to show the change in orientation and number of MODIS pixels for different rows.

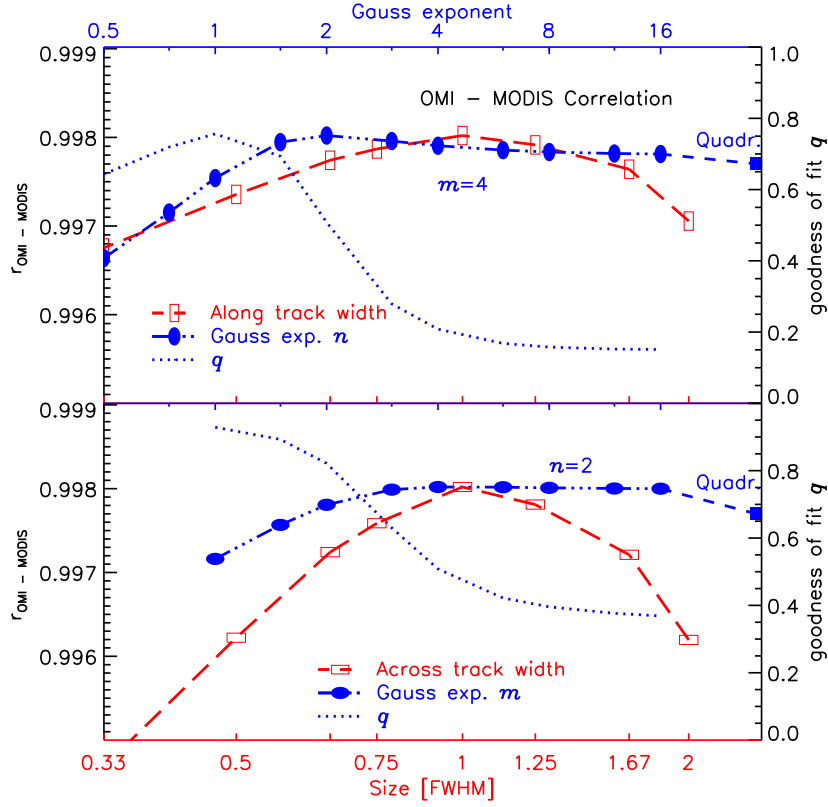


Figure 6. Pearson's correlation coefficient r for OMI and MODIS collocated reflectances in the scene of Figure 1 as a function of super-Gaussian shape and size of the assumed PSF. The blue line indicates the correlation as a function of exponent n (top panel) and m (lower panel), for fixed 75FoV corner coordinates. The red lines are the relationships for varying pixel sizes when the optimal Gaussian exponents $n = 2, m = 4$ are chosen. Note that the scales are logarithmic on both x-axes.

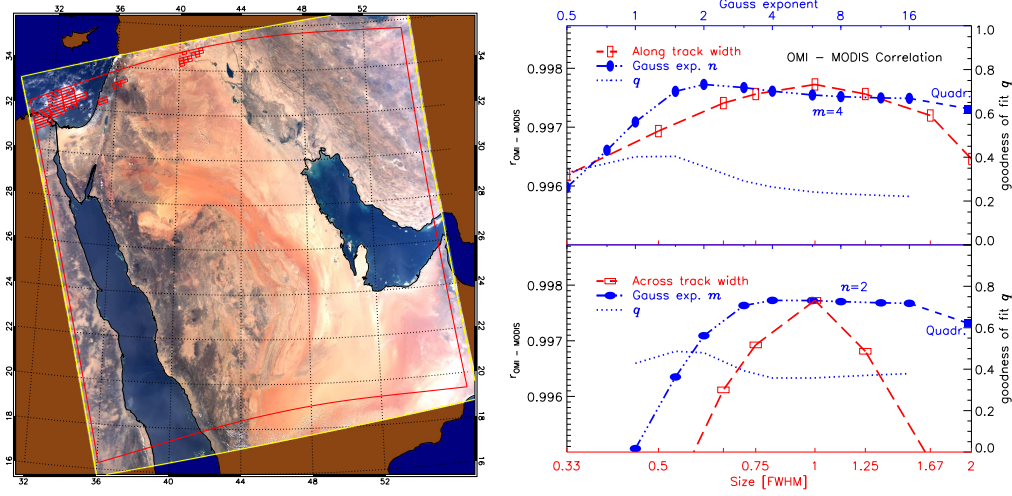


Figure 7. Left panel: MODIS RGB scene on 7 October 2008, 10:20 UTC over the the Middle East. Yellow and red lines as in Figure 1, while the individual red OMI pixels are cloud pixels that were manually discarded. Right panel: Dependence of Pearson's correlation coefficient r between the OMI and MODIS observed reflectance for the scene in the left panel as a function of super-Gaussian shape and size, as in Figure 6. The optimum in this case was found for Gaussian exponents $n = 2, m = 4$ and $1 \times 75\text{FoV}$ corner coordinates in both directions.

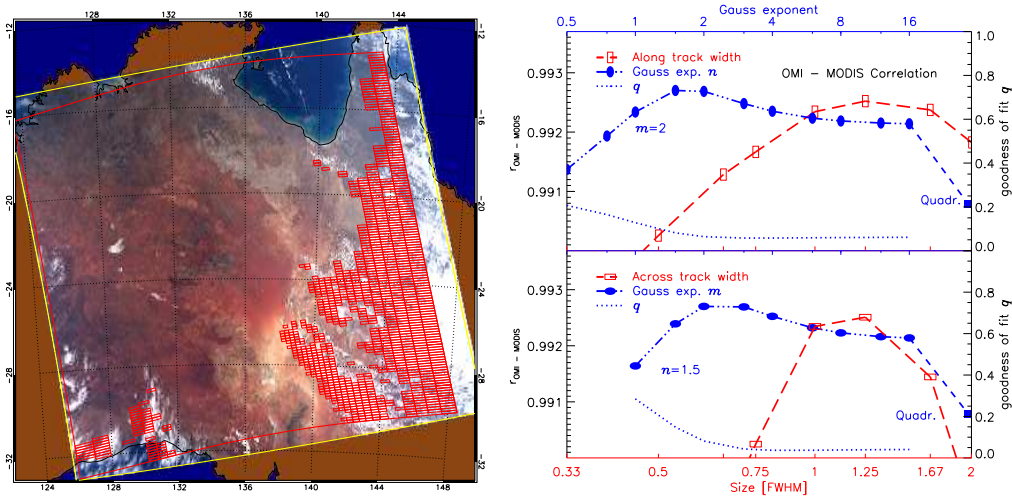


Figure 8. Same as Figure 7 on 11 October 2008, 04:45 UTC over Australia. The optimum in this case was found for Gaussian exponents $n = 1.5, m = 2$ and $1 \times 75\text{FoV}$ corner coordinates in both directions. A fit of Gaussian exponents $n = 2, m = 4$ is best for slightly larger pixels ($1.25 \times 75\text{FoV}$, red line).

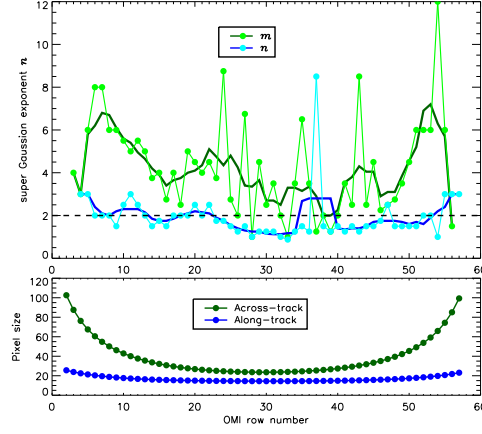


Figure 9. Super-Gaussian exponents m and n as a function of OMI pixel row, averaged over all scenes introduced in this paper. The FWHM was fixed to the 75FoV pixel sizes, shown in the lower panel, to determine the optimal exponent. The fat lines are boxcar averages using 5 points.

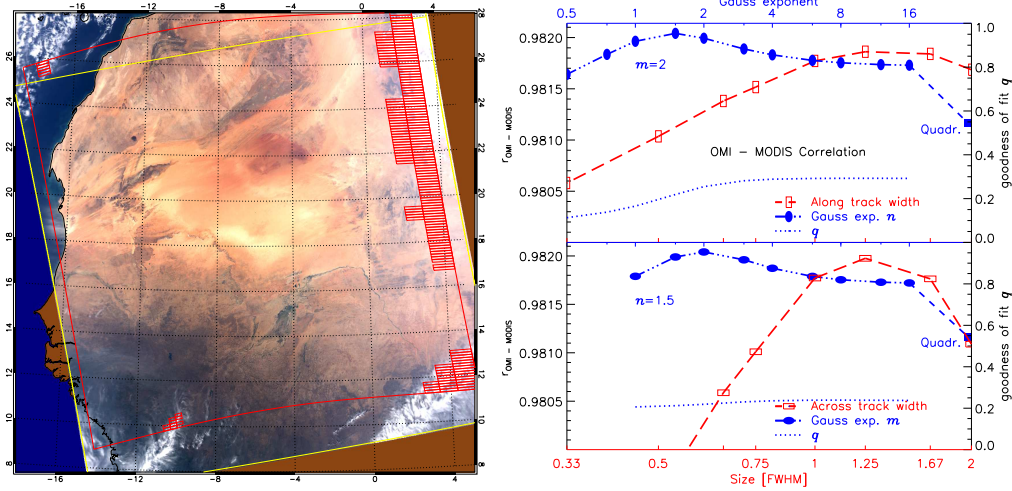


Figure 10. Same as Figure 7 on 7 January 2008, 13:45 UTC over the Sahara desert. The optimum in this case was found for a Gaussian exponent $n = 1.5, m = 2$ and $1 \times 75\text{FoV}$ corner coordinates, or $n = 2, m = 4$ and $1.25 \times 75\text{FoV}$ corner coordinates in both directions.

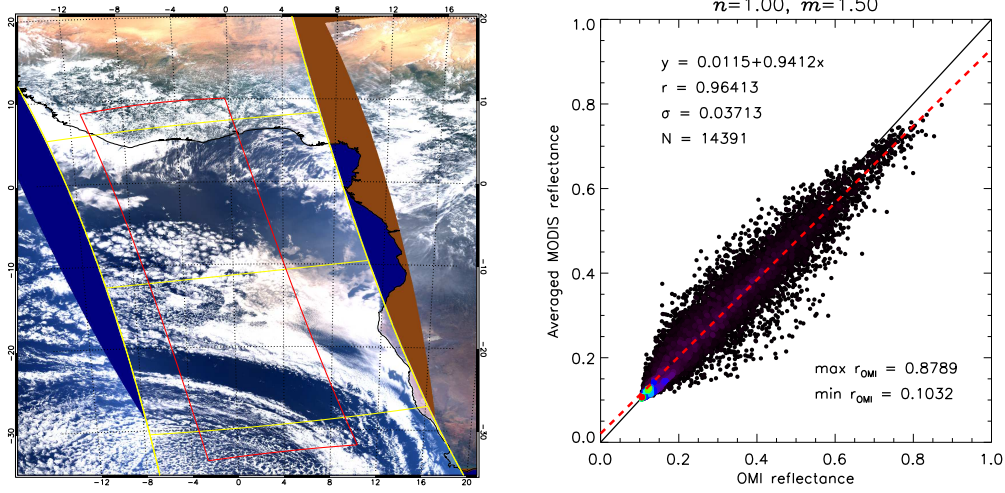


Figure 11. MODIS RGB image on 13 August 2006, around 13:33 UTC (lower part of the image). The yellow lines indicate the MODIS data granules and the red lines the considered OMI swath, which was from rows 10–50. The optimal correlation between OMI and MODIS for this scene was found for Gaussian exponents $n = 1, m = 1.5$ and 75FoV corner coordinates. The correlation for this pixel shape is shown in the right panel.

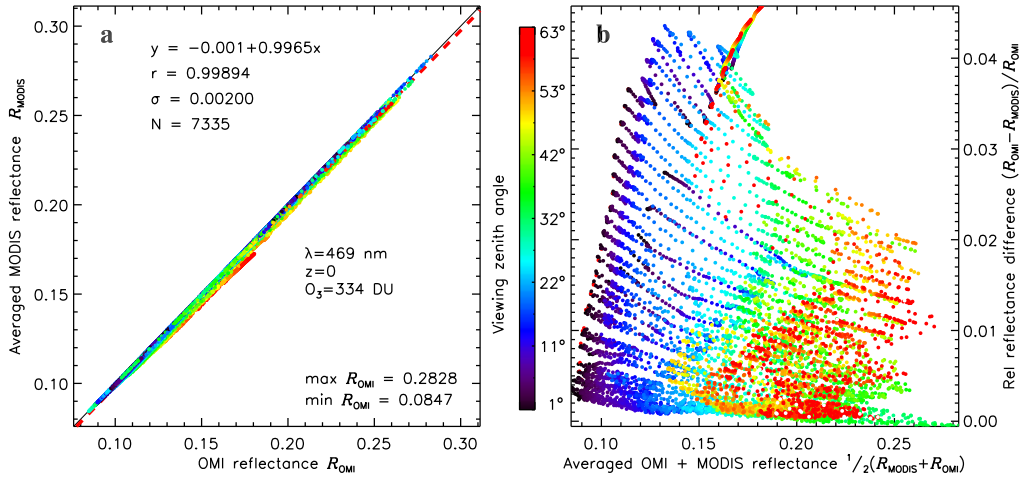


Figure 12. Left panel: Simulated clear-sky reflectances for the reference scene in Figure 1 using OMI scattering geometries (x -axis) and MODIS geometries (y -axis). The colours indicate the OMI viewing zenith angle of each simulated pixel. The reflectances were simulated at 469 nm, for a standard atmosphere reaching to sea level, and an ozone column of 334 DU. The surface albedo was varied according to a database (see text). The underlying red dashed line shows the linear fit to the simulations. Right panel: same data as in the left panel, but plotted as the relative difference between the OMI and MODIS reflectances.