A Temporally Consistent NO_2 data record for Ocean Color Work

Wayne Robinson, Ziauddin Ahmad, and Charles McClain

Ocean Biology Processing Group (OBPG)
NASA, Goddard Space Flight Center

(Wayne.Robinson@nasa.gov)

Tropospheric NO_2 measured by satellites Workshop,
KNMI, DeBilt, the Netherlands
September 10 – 12, 2007

1. Abstract

Accurate ocean color retrievals depend on the accounting for the gaseous absorption affecting the visible radiances from 412 nm. up to the Near-IR. Recently, the Ocean Biology Processing Group at NASA Goddard Space Flight Center has been working on making an NO_2 absorption correction for the visible bands with GOME, SCIAMACHY, and OMI NO2 as the data source. Differences in the NO_2 from GOME and SCIAMACHY to OMI have been seen to cause discontinuities in the retrieved water-leaving radiance (radiances from the ocean surface) and chlorophyll-a products. A correction has been developed to make a more consistent set of NO_2 measurements so that these discontinuities are reduced. The development of this correction and the results of the correction will be discussed.

2. Background

The Ocean Biology Processing Group (OBPG) at Goddard Space Flight Center has been working extensively with ocean color measurements from the SeaWiFS instrument, on the ORBVIEW-2 satellite and the MODIS instrument on Aqua and Terra to make the most accurate and consistent ocean color record possible. The main ocean color parameters consist of water-leaving radiance (Lwn), which is the radiance from the ocean surface, chlorophyll-a (chlor-a), and other atmospheric and in-water parameters. A key component of the correct processing of the data involves the removal of contributions from atmospheric aerosols and gases in the visible and near-IR bands. This part of the process is particularly important for ocean color radiances considering that approximately 90% of the radiance seen at the top of the atmosphere is due to atmospheric contributions.

The OBPG accounts for the effects of many atmospheric constituents, such as Rayleigh radiances, ozone and oxygen absorption and various aerosol types. However, recent work surveying the impact of NO_2 (Ahmad et. Al, 2007, Robinson et. al, 2007) has shown the importance of NO_2 variations upon the retrieval of water-leaving radiances and chlorophyll-a.

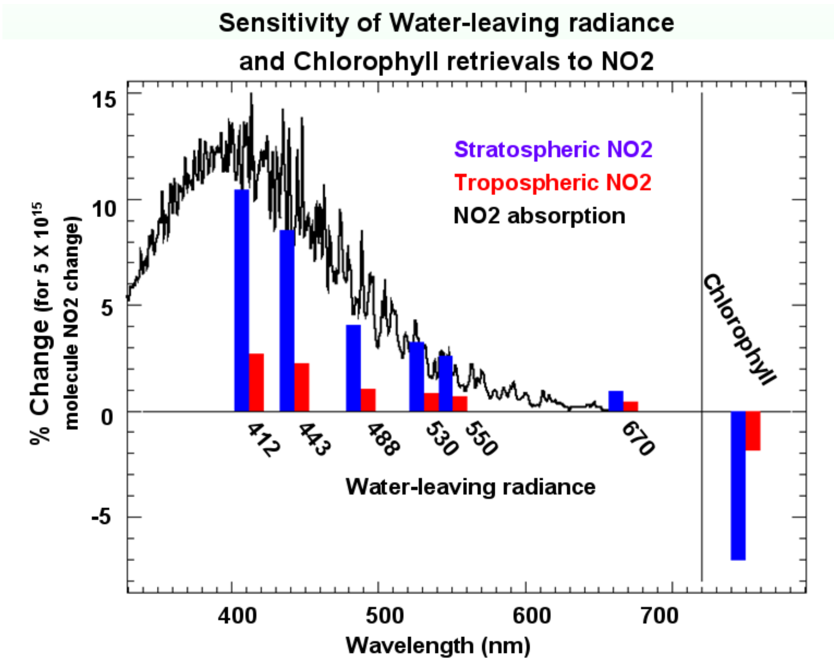

Figure 1. Sensitivity of the MODIS Aqua band water-leaving radiances and chlorophyll-a to a change in stratospheric (blue) and Tropospheric (red) NO_2 of 5 x 10^{15} molecules. The black curve is the NO_2 absorption spectra.

The sensitivity of ocean color retrievals to changes in NO_2 is shown in Fig 1. The visible bands of the MODIS Aqua instrument cover the range from 412 to 670 nm. The blue / red bars located at these wavelengths show the percentage change in the water-leaving radiances in each of the 6 Aqua bands to a stratospheric / tropospheric NO_2 change of 5 X 10^{15} molecules. Tropospheric NO_2 has a smaller effect due to the reduced amount of radiance passing through the entire atmosphere to the surface and back. The effects of NO_2 naturally are the greatest in the blue (412 nm) bands, which is near the peak of the NO_2 absorption (black line). Chlorophyll, being roughly proportional to the ratio of the water-leaving radiance in the green (550 nm) to that in the blue (412 and 443 nm), is reduced in response to an increase in NO_2.

The inclusion of NO_2 data into the operational processing involves extensive tests to assess the global and regional impacts as well as to verify that the new data source and algorithms are functioning as expected.   Testing included the processing of a significant global and temporal sample of the Aqua measurements throughout the mission (August, 2002 to December, 2006), which could then be compared to runs without the use of NO_2. Comparisons were made of the mean water-leaving radiances and chlorophyll-a throughout the mission both globally and in latitude zones. Ratios of these measurements were also used to show the relative changes.

The NO_2 fields constructed for operational processing and testing were made as monthly averages of the total, tropospheric and stratospheric NO_2 from the GOME, SCIAMACHY, and OMI instruments. When data from more than one instrument was available in a month, preference was given to data from the instrument with the higher resolution. Thus, OMI had precedence over SCIAMACHY, which ha precedence over GOME.

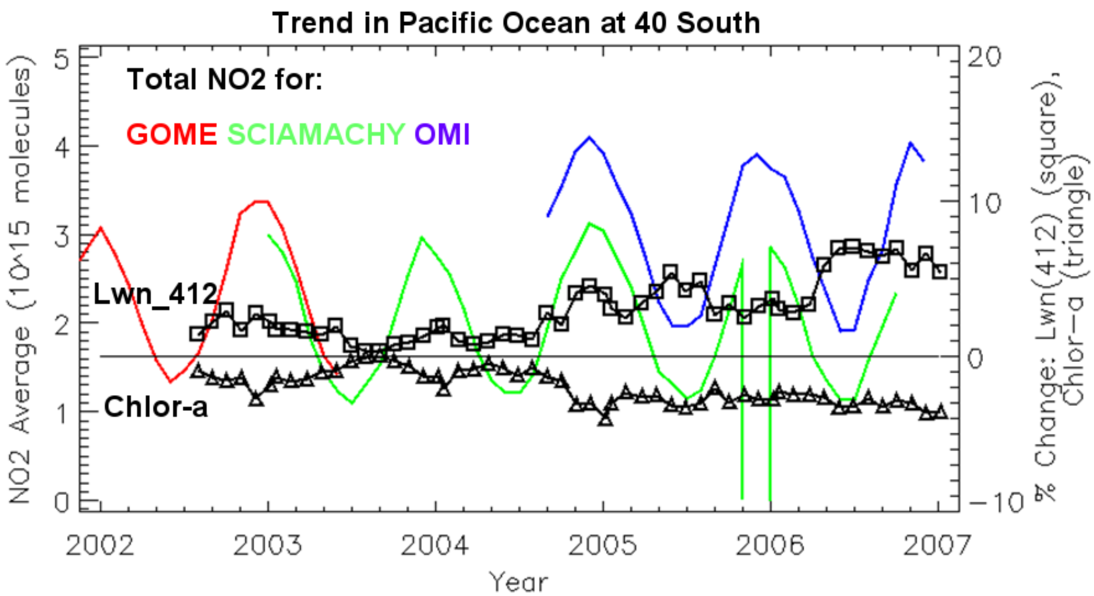

Figure 2. Effect of including NO2 absorption on ocean color retrievals. This is the temporal trend of the % change of average water-leaving radiance at 412 nm (black line with boxes) and chlorophyll-a (black line with triangles) for a zonal region of the Pacific Ocean around 40° South latitude. Also plotted are the average monthly NO_2 in the same latitude zone for the GOME (red), SCIAMACHY (green), and OMI (blus) total NO_2.

During the course of the testing of the NO_2 correction, a significant shift of the ratio of Lwn and chlor-a was observed. Figure 2 shows these trends observed in the 412 nm water-leaving radiances (Lwn_412) and in chlor-a in the 40 degree South latitude zone in the Pacific Ocean. The shift was caused by the switch of the NO_2 data source from SCIAMACHY to OMI in August, 2004. The total mean NO_2 for GOME, SCIAMACHY and OMI is included on Fig 2 to show the shift in mean NO_2 corresponding to the ratio shift. Shifts were also observed globally and in other latitude zones, but were smaller than the shift seen at 40° South.

In order to use the highest resolution NO_2 data in operational ocean color processing, it was necessary to modify the data sources to match each other. For the series here, the GOME and SCIAMACHY data was modified to match the OMI monthly data.

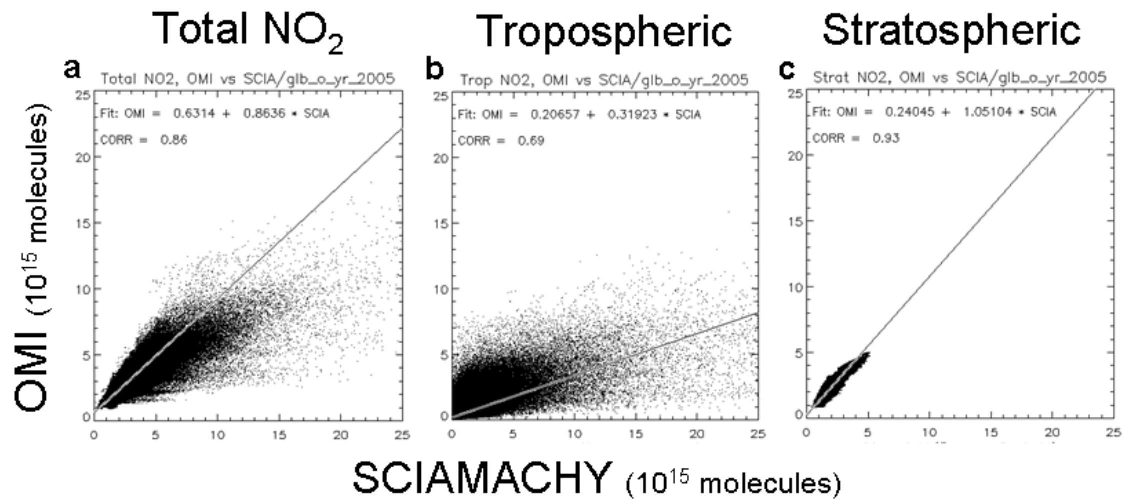

Figure 3. Scatter plots of global monthly total (a), tropospheric (b), and stratospheric (c) NO_2 for OMI vs. SCIAMACHY for the year 2005. Linear fits are plotted for each.

3. Preliminary tests: linear fit

Initially, a simple linear fit was applied to relate the monthly total, tropospheric and stratospheric NO_2 from SCIAMACHY to OMI for all the monthly data in 2005. Fig. 3 shows the scatter plots of this data and the best fit. Several shortcomings of a linear fit to the global data were found.

First, significant biases were found between the total and stratospheric NO_2 when specific latitude ranges were considered. Biases between OMI and SCIAMACHY (after the fit) varied and were the largest at 40° South latitude, where biases in total NO_2 were up to 0.5 x 10^{15} molecules. A latitudinal dependence of the correction is explored in section 4.

Next, the scatter plot of total NO_2 shows a non-linear relation between the OMI and SCIAMACHY. OMI total NO_2 does not rise as quickly as SCIAMACHY at high NO_2 values (around 10 x 10^{15} molecules and above). To address this, a non-linear fit was examined (section 5).

Last, the tropospheric NO_2 scatter plot showed little correlation. Due to this and the close relation of the total, stratospheric and tropospheric NO_2, the modified tropospheric NO_2 will be derived as the difference of the modified total and stratospheric NO_2.

4. Latitudinal dependence

When the scatter plot of OMI vs. SCIAMACHY NO_2 was performed for limited latitude ranges, it was found that the low NO2 values (from 1 – 3 X 10^{15} molecules) shifted as a function of latitude. To examine this more closely, the bias between OMI and

SCIAMACHY total tropospheric, and stratospheric NO_2 was computed for a small range of SCIAMACHY values (1.5 – 1.7 x 10^{15} molecules) and for 2 degree latitude ranges over the globe. The bias vs latitude shows a sinusoidal pattern for the total and stratospheric NO_2 (Figure 4). The bias in the tropospheric data could have an effect, but was ignored for this study.

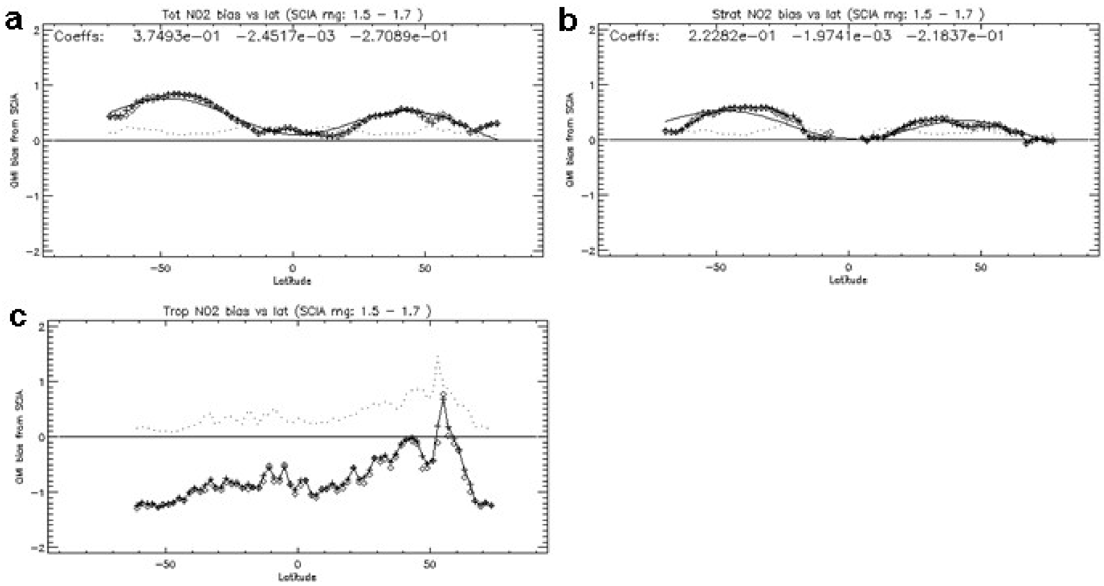

Figure 4. The latitude dependence of the OMI – SCIAMACHY bias vs. latitude (mean is the crosses and median is the diamonds) for total (a), stratospheric (b), and tropospheric NO_2 (c). Over plotted on the total and stratospheric plots is a cosine plus a linear fit.

The fit to the bias resembles a cosine of latitude plus a linear term. A fit was applied to the total and stratospheric data of the following form:

$$bias = a_0 + a_1 * latitude + a_2 * COS(4 * latitude) \qquad (1)$$

with the following coefficients:

Coeff	Total	Stratospheric
a_0	0.37493	0..2282
a_1	-2.4517 x 10^{-3}	-1.9741 x 10^{-3}
a_2	-0.27089	-0.21837

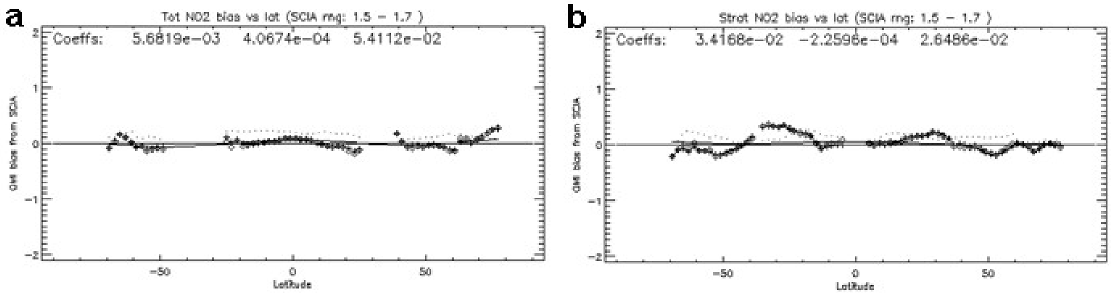

Figure 5. Same as Fig 4, but after the latitude dependence has been removed. Only the total (a) and stratospheric (b) plots are shown.

As a confirmation of the performance of this fit, Fig 5 shows the same plot as Fig 4 but with the bias removed.

This correction was also found to work well for the data ranges up to 2.5 X 10^{15} molecules (not shown). The latitudinal correction will be applied to the SCIAMACHY data as an offset.

5. Non-linear relation

Five forms of non-linear fit were applied to the latitude-corrected scatter of OMI vs SCIAMACHY. Among the fit forms tried were:

1. Quadratic fit: $y = a_0 + a_1 x + a_2 x^2$
2. Geometric fit with a constant: $y = a_0 x^{a1} + a_2$
3. Geometric fit without a constant: $y = a_0 x^{a1}$
4. Modified exponential: $y = a_0 x + a_1 (1 - a_2^x)$
5. Modified exponential with constant: $y = a_0 x + a_1 (1 - a_2^x) + a_3$

with:

x - uncorrected SCIAMACHY NO_2
y - corrected SCIAMACHY NO_2

The modified exponential fit worked best at fitting the high NO_2 and gave a relatively small y-intercept (unlike the geometric fit). Figure 6 shows the fits obtained for the total and stratospheric NO_2, plotted on the scatter plot of OMI vs latitude corrected SCIAMACHY. The fit to the stratospheric data was found to be significantly different from that for the total NO_2. Considering that the total and stratospheric NO_2 should match in many locations, it was decided that the fit for the total NO_2 would be used for the stratospheric data, but with a modified constant term to make the OMI-corrected SCIAMACHY bias be zero.

The final form for the non-linear correction was:

$$y = a_0 x + a_1 (1 - a_2^x) + a_3 \qquad (2)$$

with the following coefficients:

Coeff	Total	Stratospheric
a_0	0.29103	0.29103
a_1	5.1114	5.1114
a_2	0.80189	0.80189
a_3	-0.39714	-0.28453

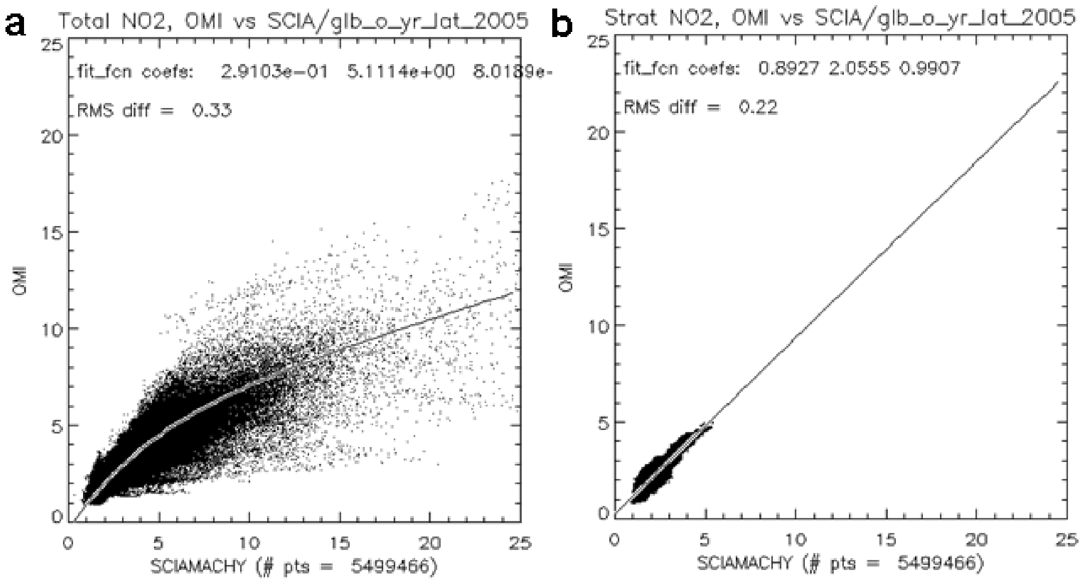

Figure 6. Scatter plots of the OMI vs. SCIAMACHY total (a) and stratospheric (b) NO_2 with the best fit lines using the modified exponential equation.

6. Results of the correction

6.1 Scatter plots

Figure 7 shows the complete set of total, tropospheric and stratospheric scatter plots for both before and after the SCIAMACHY corrections for latitude dependence and non-linearity were applied. Note again that the tropospheric data were derived from the corrected total and stratospheric data. The correction makes a much better fit for all NO2 parameters and even the tropospheric NO_2 shows higher correlation, lower RMS difference and smaller bias.

As a demonstration of the correction in latitude zones, Figure 8 shows the scatter plot of stratospheric NO_2 in the 40 S° latitude zone before and after the corrections are applied. The offset (of almost 0.6 x 10^{15} molecules) can be clearly seen in Fig 8a and the bias is substantially removed in Fig 8b.

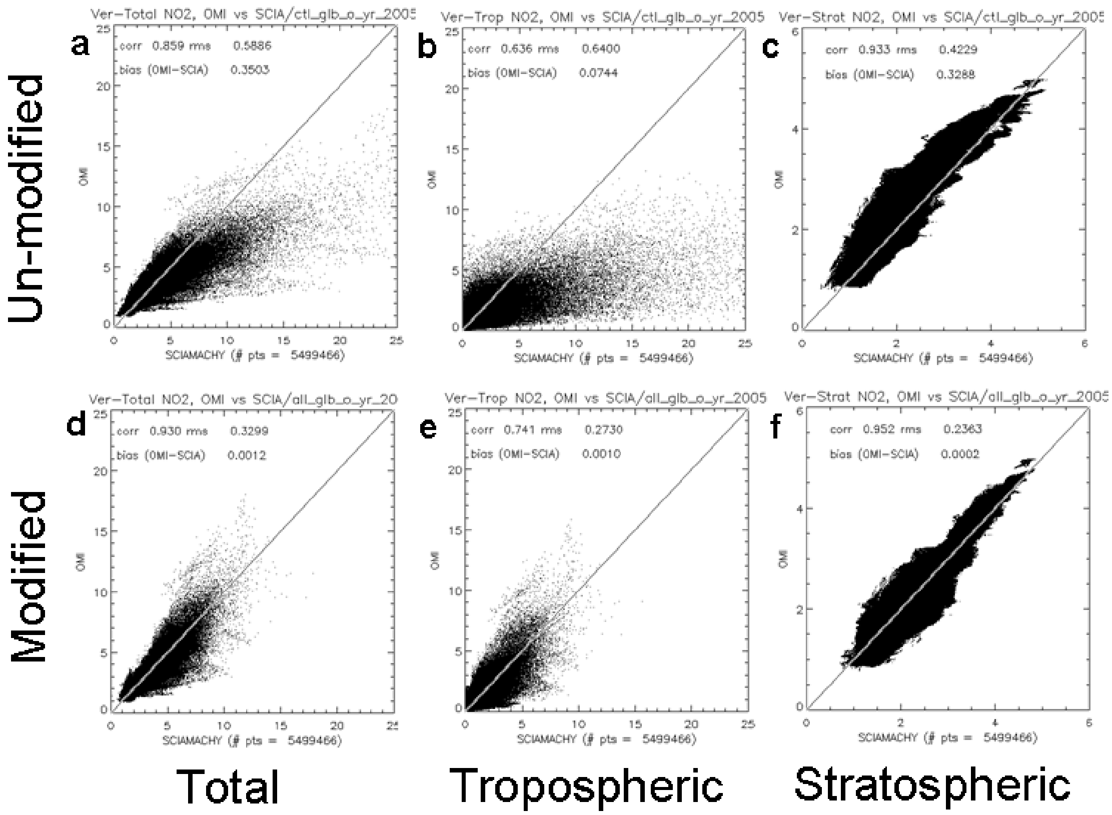

Figure 7. Scatter plots of global OMI vs. SCIAMACHY total (a, d), tropospheric (b, e), and stratospheric (c, f) NO_2 before any correction was applied (a, b, c) and after the latitude and non-linear corrections were applied (d, e, f) to the SCIAMACHY data.

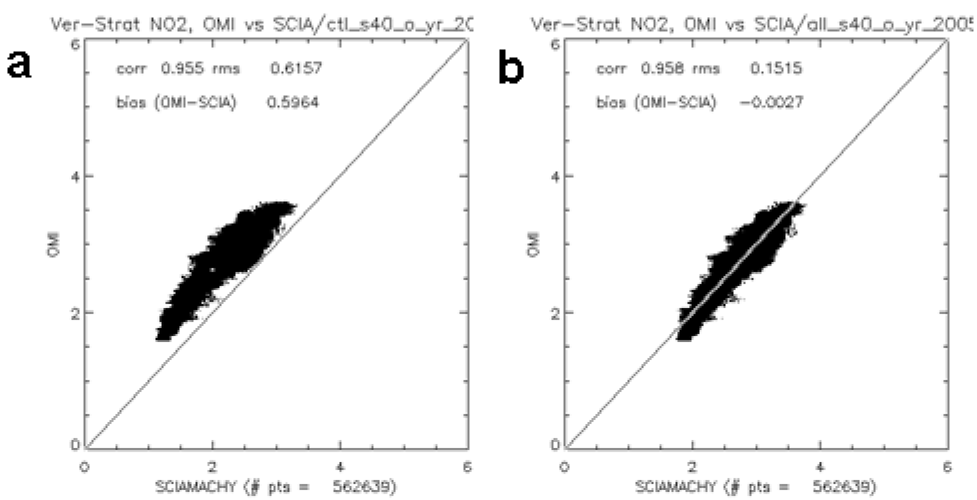

Figure 8. Scatter plots of OMI vs. SCIAMACHY stratospheric NO_2 in the 40° S latitude zone before any correction was applied (a) and after the latitude and non-linear corrections were applied (b) to the SCIAMACHY data.

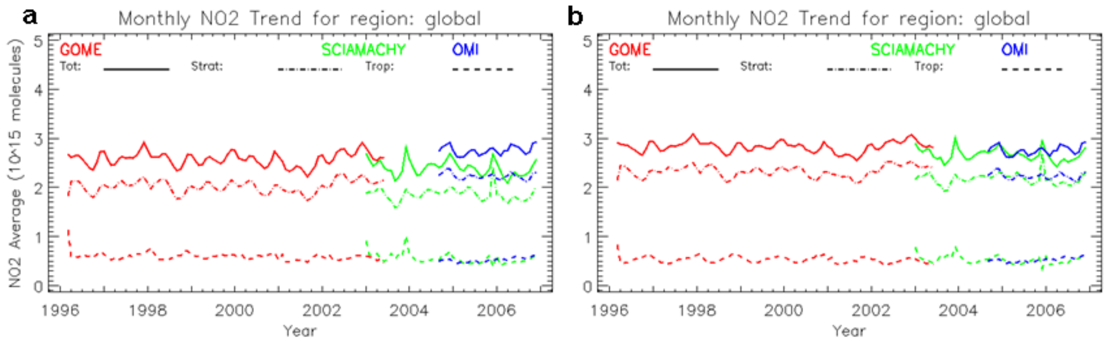

Figure 9. Global trend of the average total, tropospheric, and stratospheric NO_2 for the GOME (red), SCIAMACHY (green), and OMI (blue) instruments before the corrections were applied to the SCIAMACHY and GOME monthly data (a) and after the correction (b).

6.2. NO_2 trend

The temporal trend of the average monthly GOME, SCIAMACHY, and OMI NO_2 for the global oceans is shown in Figure 9 for before (a) and after (b) the NO_2 correction is applied to the SCIAMACHY and GOME data. The agreement for the total, tropospheric and stratospheric NO_2 is markedly improved when the correction is applied. There is a possible drift of the OMI data as compared to the SCIAMACHY, going into 2006, but more data may be needed to confirm the drift.

When the trend plot is restricted to the 45 degree South zone (Fig 10), the agreement is improved, but a difference is seen in the tropospheric NO_2 that translates into some difference in the total NO_2. This discrepancy could be due to the variable latitudinal bias seen in the latitude dependency test (Fig 4c) and could be explored more if the impact to global ocean color parameters is still evident.

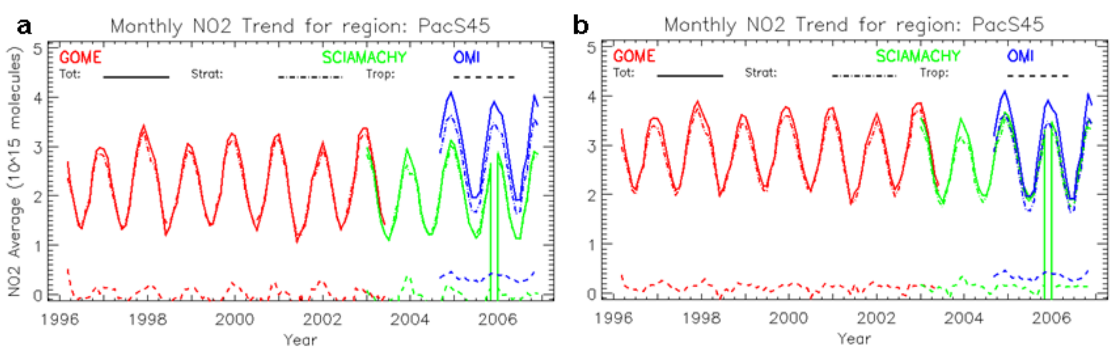

Figure 10. 40 degree south latitude zone trend of the average total, tropospheric, and stratospheric NO_2 for the GOME (red), SCIAMACHY(green), and OMI (blue) instruments before the corrections were applied to the SCIAMACHY and GOME monthly data (a) and after the correction (b).

6.3. Ocean color test scenes

We intend to perform temporal Aqua retrievals as was done to make Fig 2, but at this time, those tests are still in-progress. However, tests using the corrected SCIAMACHY NO_2 were run on a selected set of Aqua scenes. In these tests, the standard ocean color processing with NO_2 correction included was performed on 4 Aqua scenes at various latitudes, including a coastal scene with high amounts of tropospheric NO_2 and chlorophyll. Three runs were done on each scene using the OMI NO_2, the uncorrected SCIAMACHY NO_2, and the corrected SCAIMACHY NO_2. The median of Lwn_412 and chlor-a were examined for each case.

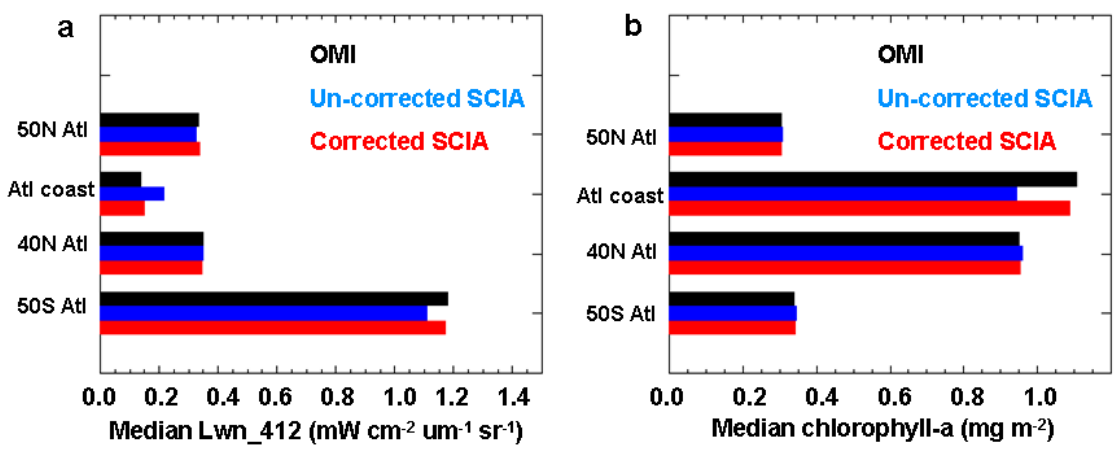

Figure 11. Median of Lwn_412 (a) and chlor-a (b) for 4 MODIS Aqua scenes. The bar colors indicate the NO_2 source used in the processing: OMI NO_2 in black, un-corrected SCIAMACHY NO_2 in blue, and corrected SCAIMACHY in red.

Figure 11 shows the results of the test runs. The median Lwn_412 and chlor-a using the corrected SCIAMACHY (red bars) agree better with the values found using the OMI NO_2 (black bars) than with the un-corrected SCIAMACHY (blue bars). For the coastal, high tropospheric NO_2 case (Atl coast), the improvement is very significant, with Lwn_412 using corrected SCIAMACHY NO_2 differing from the OMI by 7% vs. 55% when compared to the un-corrected SCIAMACHY NO_2.

7. Summary

The new corrected SCIAMACHY NO_2 should help significantly in removing the discontinuity in NO_2 seen when switching from the SCIAMACHY to OMI. It will still be necessary to perform larger temporal tests to assure that the modified record is good enough for ocean color work. The latitudinal and non-linear corrections have reduced many of the biases previously seen. However, some problems may remain that could be improved with more latitudinal corrections. Also, seasonal variations could have an effect but were not fully examined. Lastly, this work does not determine that one data source is more representative of the actual NO_2 than another. The only goal was to make a more consistent series of NO_2 that would not induce artifacts in the ocean color data.

Note that the GOME NO_2 was corrected in the same way as SCIAMACHY, and may be good enough for ocean color work. The NO_2 trends do suggest that some improvement could be made, but the effects would probably not be noticeable.

Some time in the summer of 2007, the collection 3 of OMI data will be released. This analysis will need to be done again if the new OMI data is to be used.

8. References

Ahmad, Z., C.R. McClain, J.R. Herman, B. Franz, E. Kwiatkowska, W. Robinson, E.J. Bucsela, M. Tzortziou, 2007, "Atmospheric Correction for NO_2 Absorption in Retrieving Water-Leaving Radiances from the SeaWiFS and MODIS Measurements", Appl. Optics, 46, pp 6504 – 6512.

Robinson, W.D., Z. Ahmad, B.A. Franz, S.W. Bailey, C.R. McClain, "NO_2 Data Use for Ocean Color", 2007, on http://oceancolor.gsfc.nasa.gov/staff/wayne/no2/ocrt_talk/ocrt_no2_poster_cor_no2.pdf