Empirically Corrected TOMS Earth Probe Dataset

Rich McPeters[1], Steve Taylor[2], Glen Jaross[2],
Dave Haffner[2], Gordon Labow[2], Matt Kowalewski[2]

[1]NASA Goddard Space Flight Center, Greenbelt, Maryland
[2]Science Systems & Applications, Inc., Lanham, Maryland
December 20, 2007

Important Note: *Earth Probe TOMS data after year 2000 should not be used for the calculation of long-term ozone trends because of residual instrument errors remaining even after correction.*

1. TOMS/EP Errors: Overview

The Total Ozone Mapping Spectrometer (TOMS) instrument launched on the Earth Probe (EP) satellite in July 1996 began to display significant errors in the data by the middle of the year 2000. The cause of these errors is hypothesized to be a complex problem involving the instrument's front optics, most likely due to a non-uniform degradation of the scanner mirror. The result is an instrument performance error that appears to vary with latitude and changes with time. The error can be as large as 40 DU in total column ozone, as high as 4 units in the Aerosol Index units, and up to 10% in the calculated surface reflectivity. On-board calbration methods are not capable of adequately tracking nor correcting these unexpected performance problems, and attempts to model the problem from first principles have not been successful. In the present dataset, empirical corrections have been applied to remove the bulk of the error caused by this uncertain source. Earth Probe TOMS ozone and reflectivity data for the period from July 28, 1996 through December 13, 2005 have been corrected as described in this document.

The empirical corrections applied to Earth Probe TOMS data are based on multiple internal validation techniques using geophysical data, such as tropical total ozone or minimum surface reflectivity, to detect error in the measurement. Not all methods of internal validation consistently agree. The empirical corrections made to EP/TOMS are based on those validations which improve the data under the majority of measurement conditions. Corrections to the TOMS reflectivity values and cross track dependent error in total ozone are made by adjusting instrument radiances internally using the TOMS/EP data alone. In contrast, a time and latitude dependent error in the long-term total ozone record must be corrected using information from measurements from other sources. For this, we rely on total column ozone measurements made by SBUV/2 instruments on the NOAA-14 and NOAA-16 missions. Using these data, we empirically correct the instrument radiances measured by TOMS to minimize the observed differences in ozone levels. This empirical correction has been applied to the ozone data records. At this time aerosol and SO_2 data records have not been corrected because of their greater sensitivity to instrument error.

The empirically corrected data have been compared to ground-based ozone measurements and to data from the Ozone Monitoring Instrument (OMI) aboard NASA's AURA spacecraft. Results show that the accuracy of the TOMS retrievals after the empirical corrections has increased significantly. While the corrected data are now near-trend quality, starting in mid-2000 they can no longer be considered an independent measurement of ozone and should not be used for long term trend calculation. For an example of a long term ozone data record constructed by combining TOMS and SBUV data, see data at the link: http://code916.gsfc.nasa.gov/Data_services/merged The remainder of this README describes the TOMS/EP instrument errors and empirical correction methods in greater detail.

2. The TOMS/EP Instrument and Calibration

The TOMS/EP instrument is a single monochromator that measures ultraviolet light reflected by the Earth-atmosphere system at six wavelengths with a 1 nm band-pass at 360.4 nm, 331.2 nm, 322.3 nm, 317.5 nm, 312.5 nm, and 308.6 nm [*McPeters et al.*, 1998]. The instrument employs a scan mirror to sample 35 Earth views across a track perpendicular to the satellite orbit, from west of the orbit track (sample 1) through nadir (sample 18) to east of the orbit track (sample 35). In order to observe sunlight reflected off of the in-flight diffuser plates, the scan mirror must rotate to approximately 90° from nadir. The assumption inherent in this design is that the instrument sensitivity is the same when viewing the diffusers as when viewing the Earth. The uneven change in cross-track sensor response that developed following launch suggests that the assumption of cross-track independence is false when significant optical degradation occurs. The result is that the calibration at each view angle is different from the others, and there is no way using the on-board sensor systems to track these changes. Furthermore, it appears that calibration changes derived using the solar diffuser measurements are not indicative of changes in the Earth view calibration.

The TOMS calibration system is composed of 1) on-board solar calibrations, 2) wavelength monitoring, 3) electronic gain monitoring and 4) diffuser reflectance monitoring. All four of the TOMS/EP calibration components performed well during the 10 year life of the sensor. It is a flaw in the radiometric calibration concept that has led to the problems described here.

The front optics of TOMS have degraded over time causing a complex change in the instrument's sensitivity as shown in Figure 1. Data processed using sensor corrections derived solely from the in-flight calibration system results in large errors in total ozone, aerosol index, and surface reflectivity. The magnitude of the errors depend on time, and become significant (up to 40 DU in total ozone, 4 units in TOMS Aerosol Index, and 10% in reflectivity) beginning mid-2000 when the throughput showed a sharp drop. Some anomalies in the surface reflectivity product were observed as early as 1997, but the corresponding effect on derived ozone and aerosol index remained small for several years thereafter.

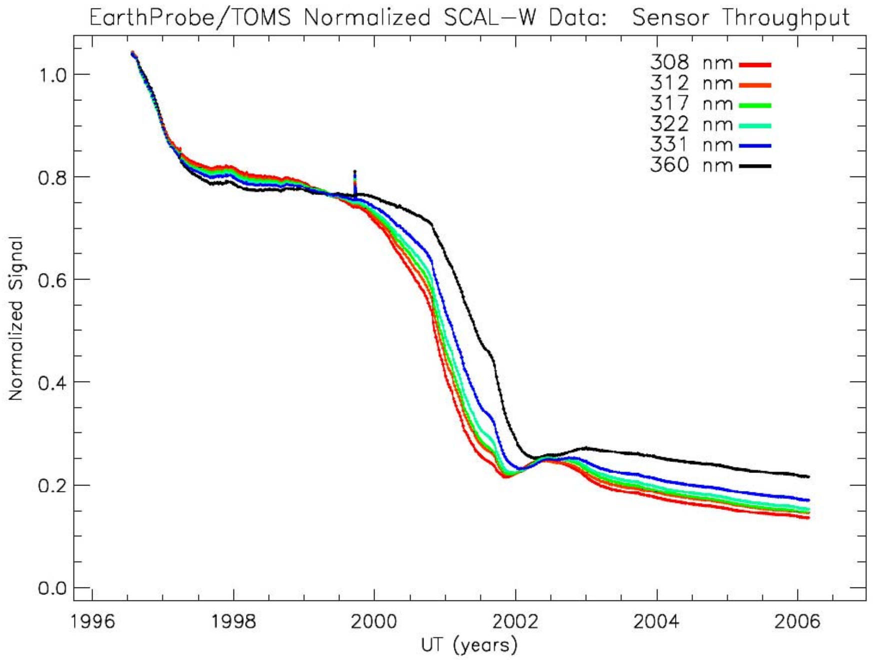

Figure 1 Sensor throughput of Earth Probe TOMS as a function of time as determined by measurements of the extra-terrestrial solar flux. Signal levels dropped by over 80% in a wavelength-dependent fashion during the mission.

The cause for the observed sensor changes is not completely understood. Degradation of the scan mirror appears to be the root cause of these changes, though other explanations are plausible. Observations of sensor response using the Mercury wavelength monitoring lamp indicate that the dramatic decline in sensor response occurred in one or more of the following: the scan mirror, the first fold mirror, the Lyot de-polarizer, or the second fold mirror. Internal calibration lamps show that the change was not in the monochromator itself or in the detector. Our best guess is that either a contaminant film developed on the scan mirror over time or else that the reflective coating on the scan mirror eroded (or both). It is very likely that, whichever process is the problem, the change was not uniform over the optical element. A uniform change in the front optics could be corrected by our standard in-orbit calibration procedures. Attempts to model the process have failed.

Over the period of time that the cross-track sensitivity was changing, the linearity of the sensor was apparently also changing. A linear response simply means that a single coefficient relates the energy of incoming photons with the signal reported by the sensor, regardless of the amount of energy. The data suggest that the TOMS/EP linearity changed slowly, in concert with the cross-track errors.

3. Overview of Empirical Radiance Correction Methods

Standard on-board radiometric “hard-calibration” systems are used to monitor and correct instrument error through multiplicative adjustments to radiance measurements. Additional methods known as “soft-calibration” have been developed to separately monitor instrument performance and corroborate the hard-calibration derived changes by tracking a particular geophysical quantity under conditions of evaluation. Soft-calibration techniques vary, and internal consistency among them can be used as corroborative evidence of radiometric calibration error. These internal validation methods have been used historically to make corrections to TOMS total ozone for earlier TOMS and SBUV missions, and more recently for OMI.

Hard-calibration has proven inadequate in addressing TOMS/EP instrument errors, and the multiple internal soft-calibration validation tests give inconsistent results. The instrument error is therefore correctable only through more empirical means. This new TOMS/EP empirical calibration derives from soft-calibration approaches, but differs because a multiplicative radiometric calibration correction would not remove all the error. Instead, the data have now been corrected by removing those errors which affect a larger fraction of the data. Under some observational conditions error is not removed, and in some cases it marginally increases (see section 3.1a, for example).

Empirical techniques are used to derive radiance corrections as a function of 1) cross-track scan position, 2) solar zenith angle, 3) wavelength and 4) time. For only the trend in ozone , measurements from SBUV/2 instruments on NOAA-14 and NOAA-16 are used to stabilize the TOMS/EP calibration. After calibration using these empirical methods, standard soft-calibration techniques can be used to characterize residual instrument error that empirical calibration did not address.

3.1 Surface Reflectivity Corrections

a) Internal Cross-track Surface Reflectivity Correction

The Version 8 TOMS total ozone algorithm [*Bhartia and Wellemeyer*, 2004] produces a surface reflectivity product that is derived from TOMS measurements at 331 nm. Significant errors first appeared in the 331 nm reflectivity data in 1998 at low reflectivities and became evident at high reflectivities by 2001. The errors have a strong cross track scan position dependence. Our first step in correcting the TOMS/EP data is to characterize the departures of the 331 nm minimum land surface reflectivity from a global value of 1.5% determined from the first year of TOMS/EP data, whose calibration we believe to be good. Low reflectivity data are selected for use in this internal validation because the ozone and aerosol index retrievals are more sensitive to reflectivity errors at low reflectivities than over brightly reflective surfaces. Figure 2 shows the results of these minimum reflectivity land validations, as well as measurements of reflectivity changes over ice in 1997, before instrument errors grew apparent, and in 2001 when the errors were clearly apparent.

Analyses of TOMS/EP low reflectivity 331 nm data are used to identify absolute radiance error and make empirical radiance corrections to all TOMS wavelengths using our theoretical knowledge of the sensitivity of radiances to surface reflectivity. These corrections are wavelength independent. The dataset is processed and corrected successively to account for weak ozone absorption until results converge to a final correction. Figure 3 shows data similar to those in Figure 2, with the final empirical cross-track radiance correction applied to correct for reflectivity error. Figure 4 on left shows a sample of the cross-track corrections effectively applied to 331 nm reflectivity for year 2003.

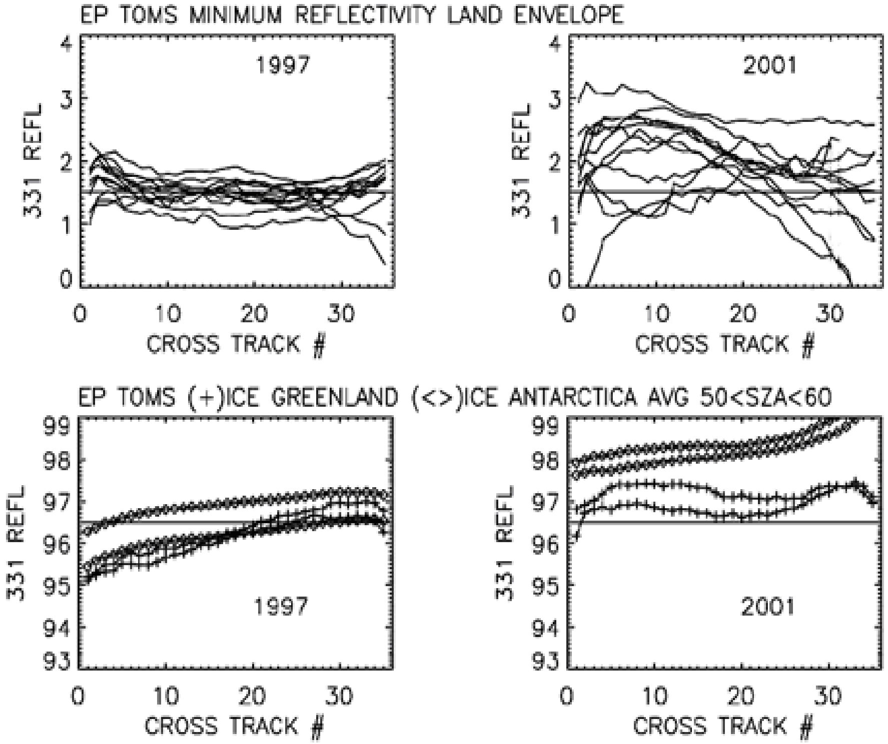

Figure 2. Global monthly minimum reflectivity over land (top) and monthly average reflectivity for Greenland and Antarctic ice at moderately high solar zenith angles (bottom) for 1997 and 2001 as a function of instrument cross-track scan position.

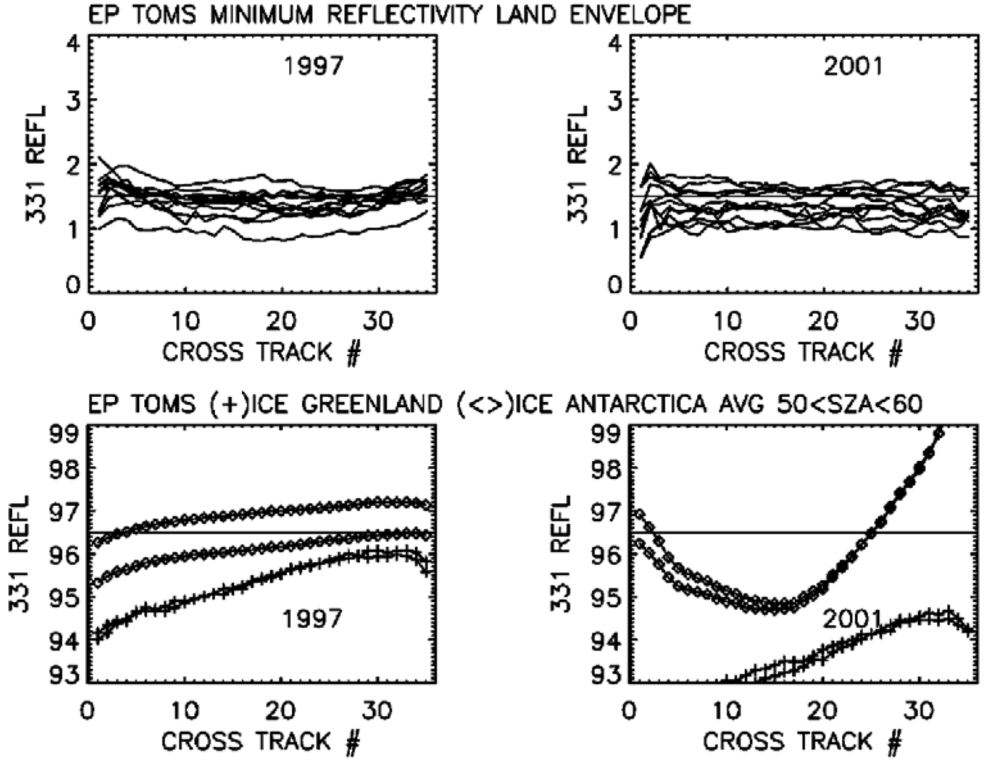

Figure 3. Same as Figure 2, but after empirical correction of cross-track reflectivity error.

Note that the correction based on evaluation of low reflectivity data imparts an *increase* in error for data retrieved over the high reflectivity ice surfaces, as seen in Figure 3. This trade off is deemed acceptable since the ozone calculation is more sensitive to reflectivity error in low reflectivity conditions, and ozone is the primary focus of these empirical corrections.

b) Internal Reflectivity Correction for Solar Zenith Angle Dependence

After cross-track empirical corrections are applied, further analysis over land and ice show that the reflectivity error increases with time and solar zenith angle, and are essentially similar at all cross-track positions. We remove this error with a radiance adjustment method similar to the one described for cross track dependent errors. Data over ice are used for solar zenith angles exceeding 55°, while data over land are used for lower solar zenith angles, again using an assumed minimum surface reflectivity of 1.5%. Examples of the final solar zenith angle- dependent empirical radiance corrections to 331nm reflectivity are show in Figure 4 on the right. The total reflectivity correction is the sum of the solar zenith angle corrections and the cross track corrections.

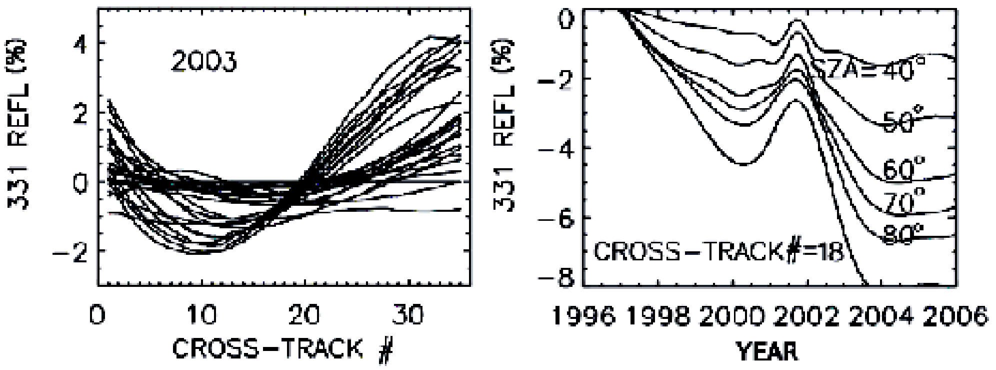

Figure 4. Average empirical radiance adjustments applied to correct TOMS/EP reflectivity as a function of cross-track for all months in 2003 on left, and as a function of solar zenith angle for the nadir (#18) scan position on right. The total reflectivity correction is the sum of the solar zenith angle corrections and the cross track corrections shown here. Corrections are expressed in reflectivity (%) for ease of interpretation, rather than in radiance, as the corrections are applied.

3.2 Total Ozone Corrections

a) Internal Cross-track Total Ozone Correction

By the summer of 2000 the total column ozone retrievals began to exhibit scene-to-scene differences large enough to be obvious in the daily global images. This cross-track scan dependence is quantified by assessing low reflectivity data between 15°N and 15°S. In this region total ozone is known to be spatially homogenous on average, so intrinsic geophysical variation across the scan track is small, as shown in Figure 5 on left. The cross track changes identified in this region are attributed to instrument error and are characterized relative to an arbitrarily referenced scan position. Cross track changes in total ozone vary in time as well, in some cases dramatically. Figure 5 shows the development of total ozone error as a function of cross track position, showing that it was small for the 12 months of 1997 (the left plot), but was large in 2001 (the right plot).

This error is not directly removed from the ozone data. The TOMS ozone retrieval is based on the ratio of the normalized radiance at a pair of wavelengths, one considerably absorbed by ozone, and the other only weakly so. Therefore errors in total ozone can be attributed to a change in this relative radiance due to instrument error. The spatially non-homogenous accumulation of contaminants on surfaces of the instrument's front optics may be responsible for the scan angle dependent nature of this effect, however the

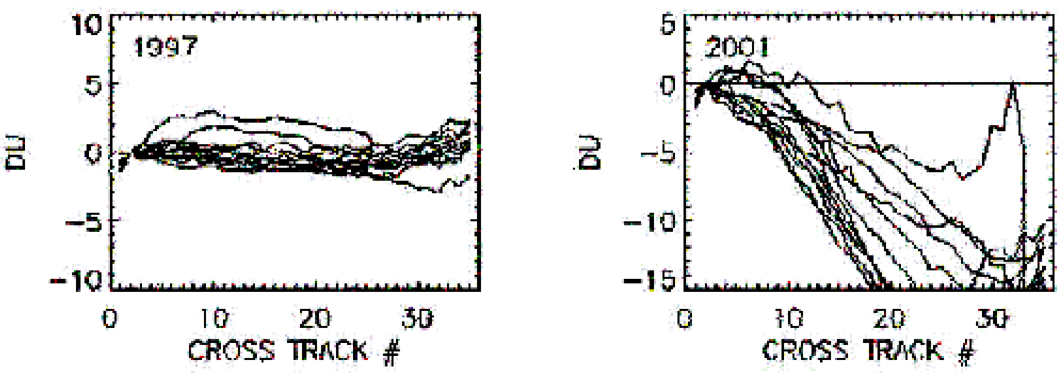

Figure 5. Results from the internal cross-track ozone validation described in the text for 1997 and 2001. Data in 1997 show little scan dependence compared to 2001. Each line represents monthly averaged ozone values from the algorithm B-pair (318 nm and 331 nm) measurements over land from 15 N-15 S and with reflectivity less than 10%. Cross-variations shown here have been normalized to cross-track position 2.

mechanism is not entirely understood. Nonetheless, this cross track error in the radiance measurements is substantially corrected by adjusting radiances at the ozone absorbing wavelengths. The radiance adjustment needed to remove the cross track error can be accurately estimated from radiative transfer calculations. Corrections are applied to the TOMS/EP data in this manner. An example of these corrections for several months in the 2003 is shown on the left in Figure 6.

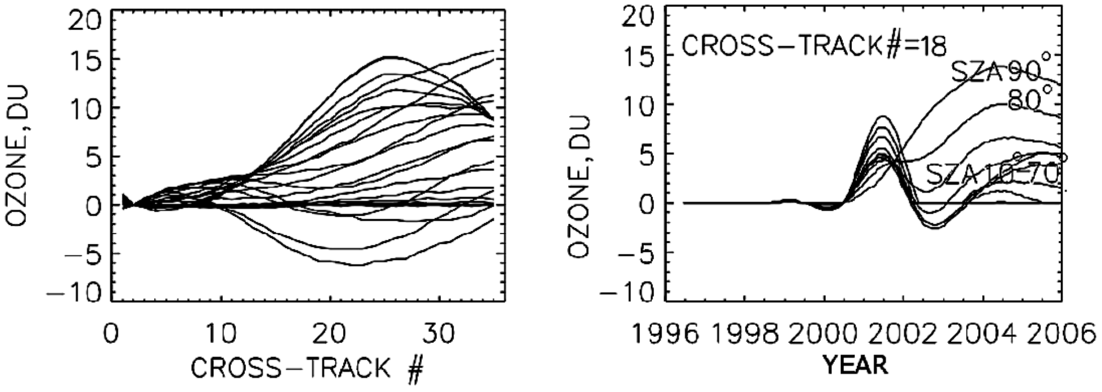

Figure 6. Cross-track empirical corrections to B-pair (318 nm and 331 nm) total ozone for all 12 months in 2003 on the left. On the right, the time dependent empirical corrections for B-pair ozone applied as a function of solar zenith angle.

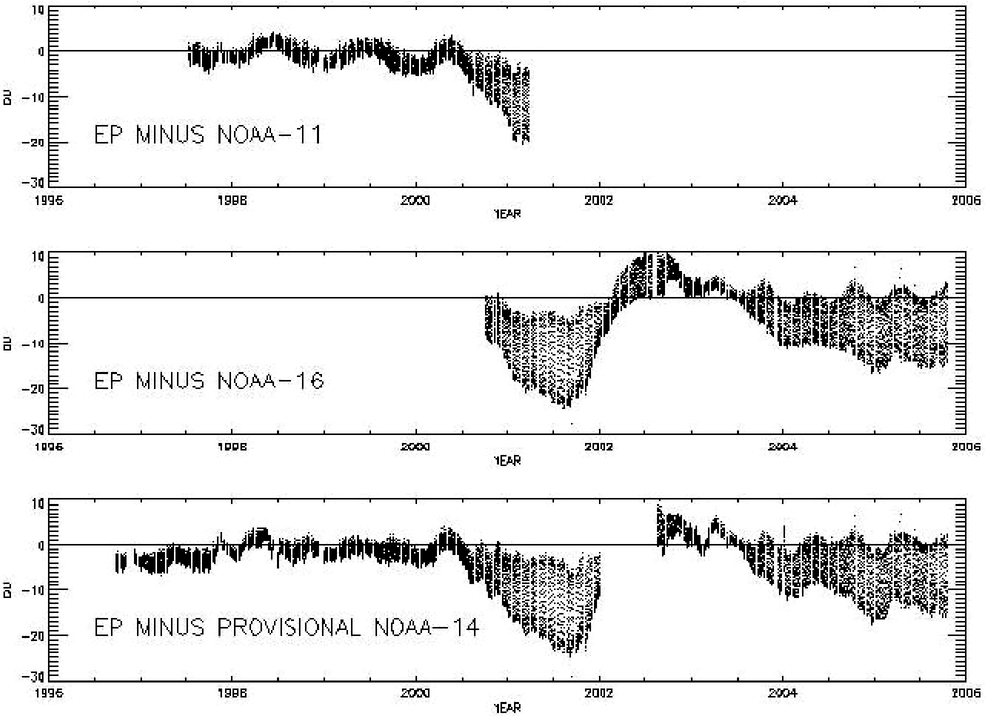

Figure 7. Weekly differences between pre-corrected (normal in-flight calibrations applied) TOMS/EP total ozone for the ± 2.5° latitude zone and measurements from SBUV/2 on NOAA-11, 14, and 16 . Vertical spread in the data show variation in the difference across the 35 TOMS scan positions compared to the averaged, nadir-only SBUV/2.

b)Correction for Trend Error in Total Ozone Using External Data Sources

After the TOMS/EP radiances are corrected to remove cross track error in total ozone, the TOMS/EP total ozone data have significantly different ozone trend with time compared to total ozone measurements made by SBUV/2 instruments aboard NOAA-11, 14 and 16 (Figure 7). These NOAA instruments have comparatively stable calibrations and thus are a reliable reference against which to measure TOMS/EP. Differences are found to vary as a function of solar zenith angle as well as time (Figure 8, top). These differences in ozone trends are characterized as error and removed by again empirically adjusting the radiances of the ozone absorbing wavelengths so that trend in the TOMS data agrees better with the SBUV/2 measurements (Figure 8, bottom).

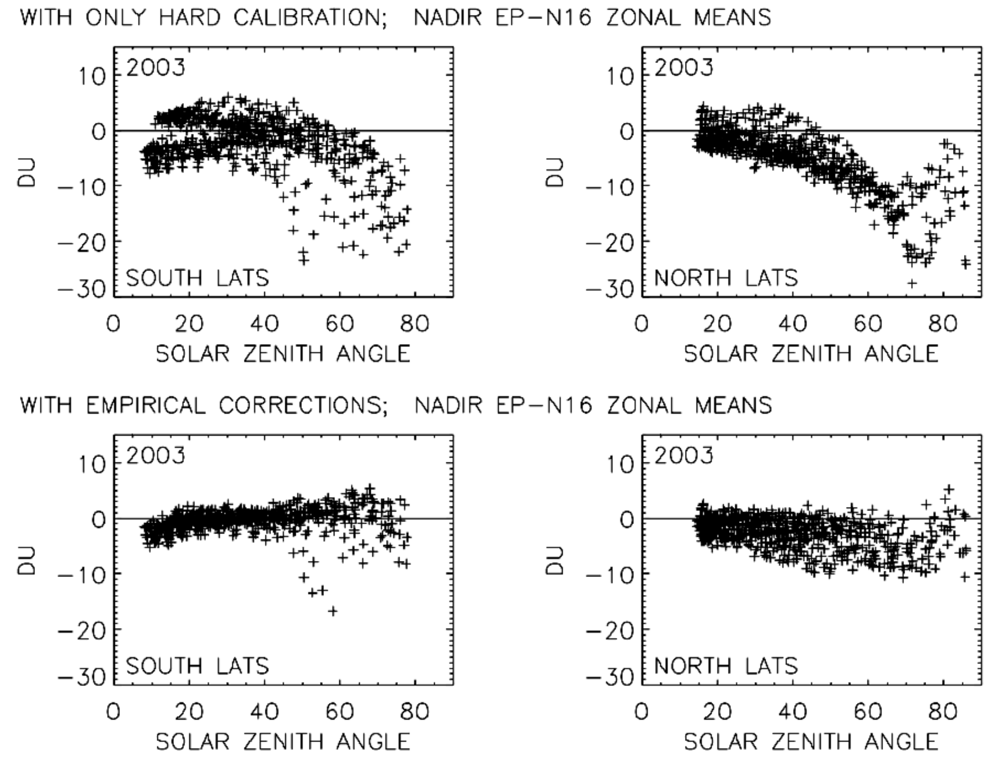

Figure 8. Total ozone differences between TOMS/EP and NOAA-16 SBUV/2 in 2003 as a function of solar zenith angle with in-flight radiometric calibration applied (top) and after empirical radiance corrections based on these data have been applied (bottom).

The use here of SBUV/2 data draws in an external source of information to the TOMS/EP measurements and therefore makes them no longer an independent measurement source. The corrected data compare much better with SBUV/2 data on which the external corrections are based (Figure 9). Note both the decrease in trend error relative to the SBUV/2 instruments after 2001, and the narrowed vertical spread in the data demonstrating substantial correction of the cross track error in ozone. Figure 10 shows the improved comparison of the corrected EP data (bottom plot) with a set of 30 independent ground based measurements and consistency with OMI on EOS-Aura.

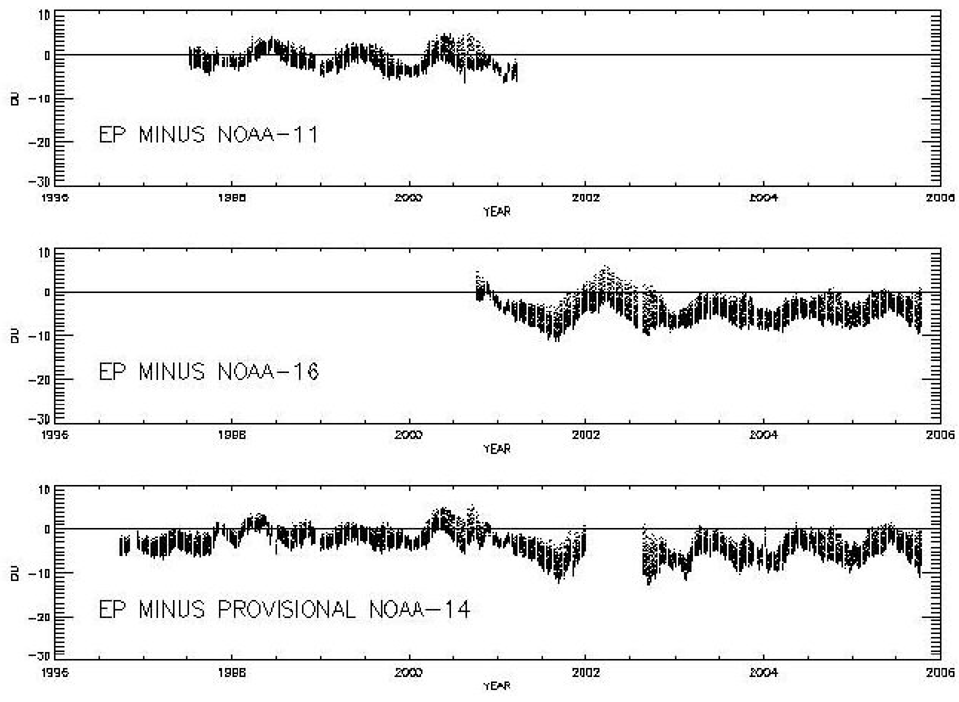

Figure 9. The same comparison as in Figure 7 between TOMS/EP and SBUV/2 data ± 2.5 degrees of the equator, but after TOMS/EP radiances have been empirically corrected.

4. Remaining Errors in Total Ozone and Aerosol Index

The remaining errors in TOMS/EP total ozone are not symmetric in the northern and southern hemisphere. Furthermore, there may be increased ozone error at the extreme off-nadir positions at higher solar zenith angles. These extreme data are not generally included in the production of the TOMS level 3 gridded data product.

The final empirical corrections to the radiances for the wavelength pair used to compute the aerosol index (331 nm and 360 nm) are relatively small; at most 1 AI unit. However in the years after 2000, contemporaneous with other evidence of instrument degradation, a systematic anomaly is observed in the aerosol index over water surfaces and nearby land. The anomaly appears in the 2003 plot over cloud free equatorial Pacific Ocean as determined by minimum 331 nm reflectivity (Figure 11). The expected signature of sea-glint over water is seen in earlier years, but is increased, broadened, and shifted towards the right of the scan (westward) in the 2003 data sample. Over low reflectivity land and bright clouds such distortion is minimal. However, the aerosol index anomaly is seen in measurements over land surfaces closely neighboring glint affected water surfaces.

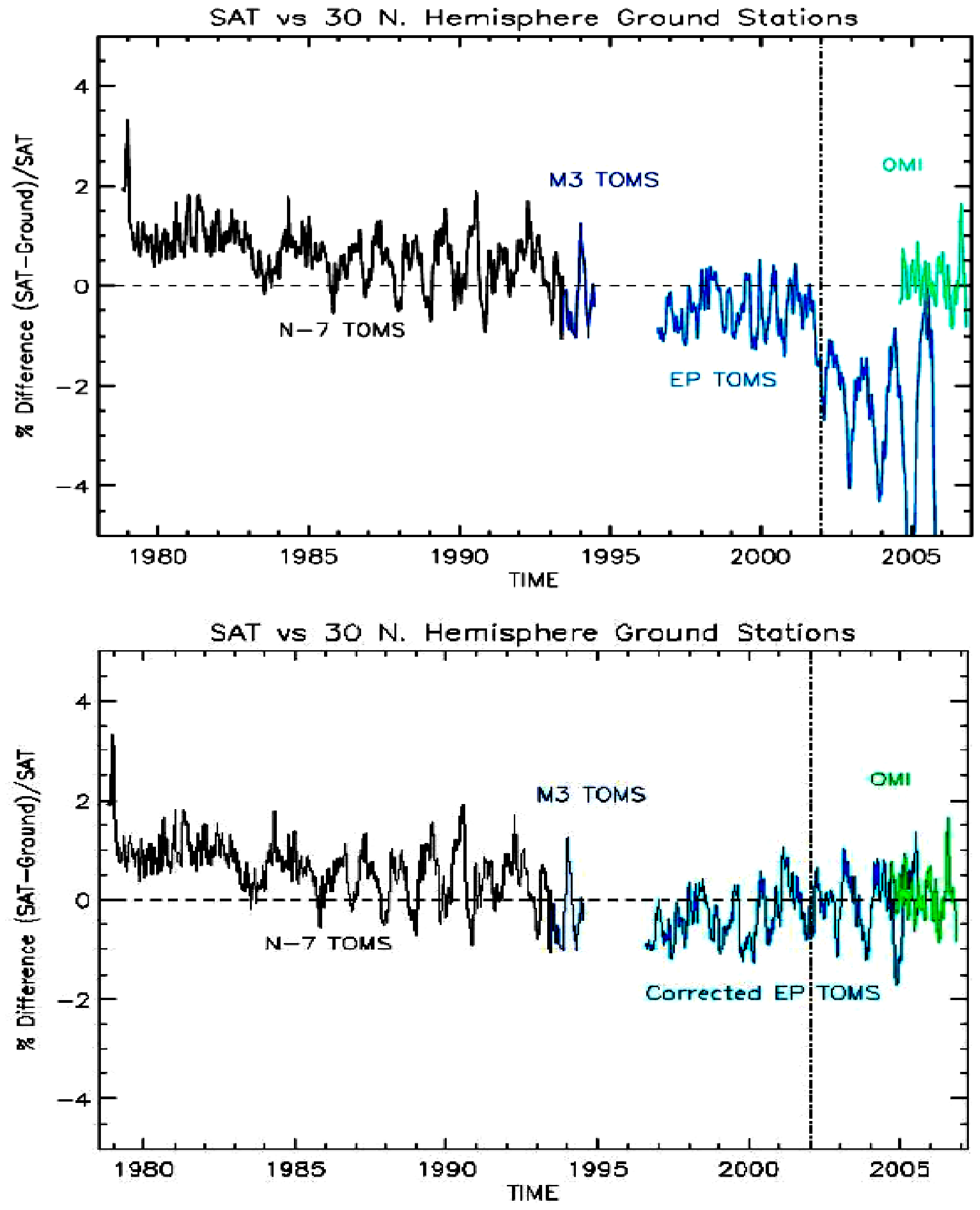

Figure 10. TOMS and OMI total ozone compared with 30 Northern Hemisphere Dobson and Brewer ground measurement with differences expressed in percent, showing TOMS/EP data before (top figure) and after (bottom figure) the data have been empirically corrected.

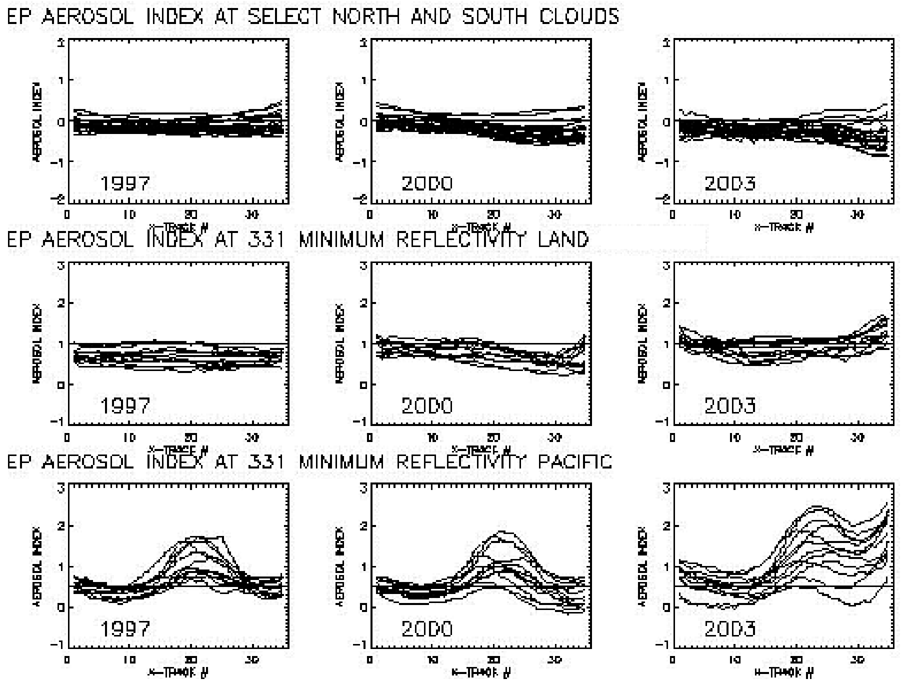

Figure 11. Three validation tests showing changes in the scan dependence of the TOMS/EP Aerosol Index after all empirical corrections are applied. Each line represents an averaged month of data. These first two rows, showing data over clouds and low reflectivity land, show little scan dependence. The bottom row shows the systematic anomaly associated with sea glint that remains in the corrected data.

References

Bhartia, P. K. and C. G. Wellemeyer, 2004, TOMS-V8 Total O3 Algorithm*, Version 8 TOMS Algorithm Theoretical Basis Document*, pp. 8-23, http://jwocky.gsfc.nasa.gov/version8/v8toms_atbd.pdf

McPeters, R. D., *et al.*, 1998, Earth Probe Total Ozone Mapping Spectrometer (TOMS) Data Products User's Guide, *NASA Technical Publication 1998-206895*, National Aeronautics and Space Administration, Goddard Space Flight Center, Greenbelt, Maryland.