Description of POAM III Version 4 Retrievals

Contents:

I. Summary of Algorithm Changes

A complete description of the POAM III version 3 retrieval algorithm, and accompanying error analysis, is given in Lumpe *et al*., [2002] (hereafter referred to as L02). The version 4 algorithm does not differ in any fundamental sense from that description, but a number of improvements have been implemented, which are summarized in this section. The primary improvements made in the version 4 algorithm involve changes in the level 1 algorithms which determine the instrument pointing information. Accurate pointing and altitude determination is the most challenging aspect of deriving atmospheric optical depth profiles from the POAM radiance measurements. During the lifetime of POAM, there has been some instrument degradation that was unexpected and not accounted for in the version 3 algorithm. In particular, it was necessary to increase the tracking gain in the elevation servo loop, which resulted in increased jitter in the tracking motion during an atmospheric scan. Also, the potentiometer that monitors the elevation motion has experienced increased nonlinearity over the mission life. These degradations have led to an increase over time in the noise and potential biases of the instrument's absolute pointing information. This of course resulted in increased noise and biases in the version 3 retrievals. Most affected were the water vapor and aerosol extinction products, because they are represent weak extinction signals and are derived primarily from the long wavelength channels. These channels are optically thin and therefore very sensitive to small pointing errors. The version 3 validation papers that have been published generally used data from the first two or three years of the mission, during which the version 3 retrieval was performing best.

The version 4 algorithm changes are primarily aimed at compensating for these problems. Specific improvements include introducing additional smoothing of the level 0 radiances to decrease the impact of tracking jitter. The smoothing is done on the native 18 Hz data grid before altitude binning to the standard POAM 1 km grid. The smoothing has a vertical scale of 1 km or less, and therefore does not degrade the effective vertical resolution of the retrievals. The calibration of the potentiometer, which relates the optical head movement to changes in altitude, has also been improved, making it less susceptible to errors due to changing potentiometer nonlinearity. Because of the increased problems with the elevation potentiometer, a significant effort was made to reduce the overall dependence on the potentiometer data in deriving the transmission algorithms. As with version 3, the potentiometer data is used to determine instrument pointing only at the lowest altitudes of each scan. At higher altitudes, the pointing is determined selfconsistently by maintaining the expected optical depth ratios between Rayleigh-dominated channels. This method has been improved in version 4, allowing it to be used down to about 26 km (about 8 km lower than in version 3).

One significant change made in the level 2 species inversion algorithm for version 4 is the parameterization used to constrain the spectral dependence of the aerosol optical depth (δ). All previous versions, for both POAM II and III, assumed a quadratic polynomial in $\ln \delta(\lambda)$ for the spectral inversion [see L02]. The version 4 algorithm now uses a simple quadratic fit to $\delta(\lambda)$ directly. This removes a major source of nonlinearity in the spectral inversion and leads to a faster and more robust species separation without significant loss in accuracy. It also eliminates occasional problems with retrieval convergence that occurred with the nonlinear form.

Finally, the water vapor line transition parameters used to compute the effective absorption cross sections in version 4 are taken from the HITRAN 2000 data base. This is a change from version 3, which used the HITRAN 96 line parameters with the 14.4% correction (line strength increase) in the 940 nm absorption band reported by Giver *et al.* [2000]. This spectroscopic change alone results in a slight increase in the retrieved water vapor. The magnitude of the increase is generally a few percent above 20 km and goes to zero at lower altitudes.

The changes introduced in version 4 have resulted in a significant improvement in the precision and long-term consistency of most of the POAM retrieval products, particularly the water vapor. The precision of the version 3 water vapor retrievals degraded over the life of the mission as a direct result of the increased pointing uncertainties. This has been largely eliminated in the version 4 retrievals. The variability in version 4 (in terms of weekly retrieval standard deviation) is greatly reduced, and shows no significant long term trend in the minimum summertime periods.

II. Version 4 error bars

The version 3 error analysis described in L02 has been repeated for the version 4 retrievals. A total error bar for each retrieved species profile is archived in the version 4 data files. This error is the root mean square (rms) combination of three error sources:

1. A total random error obtained from the theoretical error analysis (dominated by measurement noise, random altitude registration errors, and radiance normalization errors).

2. Errors due to improper removal of sunspot artifacts.

3. Aerosol feedback errors in gas retrievals due to extreme aerosol loading.

As described in L02, the latter two error sources are difficult to characterize, and empirical analyses were developed to correlate increased random retrieval error with both sunspot presence/magnitude, and aerosol loading. This analysis has been repeated for the version 4 retrievals to produce the sunspot and aerosol contamination error components used in the calculation of the total error bars.

Large sunspots can cause systematic “S-shaped” artifacts in the transmission profiles, which then propagate into the retrievals at the altitudes where the instrument field of view encounters the sunspot. High aerosol extinction increases the random error of all the gas retrievals because the signal to noise (gas optical depth to aerosol optical depth) ratio is decreased, making it more difficult to accurately separate the aerosol and gas components. Aerosol contamination is generally only a problem in the presence of PSCs, and is therefore much more common in the southern hemisphere than in the northern hemisphere (because of the much larger number of PSCs observed in the South).

These errors primarily impact the H_2O and NO_2 retrievals, in that order. The aerosol retrievals are occasionally affected by large sunspots, while O_3 is essentially immune to both of these effects.

III. Version 4 data quality flags

Although these effects are factored into the archived error bars, it is sometimes difficult to screen for data potentially corrupted by sunspot or aerosol effects using only the total error bars. This is primarily because the distribution of sunspot retrieval errors tends to be non-Gaussian. That is, errors at the several sigma level tend to occur much more often than expected from a Gaussian distribution. Therefore, in addition to providing the sunspot and aerosol statistical error bars, we flag points with potentially large sunspot or aerosol contamination, based on the statistical error value.

The value of the sunspot and aerosol errors used to determine the data screen values was determined empirically using the same technique described for NO_2 in Randall *et al.* [2002]. This procedure is necessarily somewhat arbitrary and represents our best estimate of a trade off between avoiding false negatives (contaminated data not flagged) while minimizing false positives (flag data which is not contaminated).

One final scenario can occur in the POAM retrievals which can result in increased random retrieval error in H_2O and NO_2 only. In the presence of an optically thick type 2 PSC (ice cloud) the POAM sun tracker exceeds its minimum tracking threshold and the scan will terminate higher in the atmosphere than a normal scan, typically 1 to 2 km above the cloud layer. We call this a “high Z_{min}” event, because the minimum retrieved altitude for the occultation (z_{min}) is significantly outside the range of all clear-sky events. All occultations that terminate above 16 km are flagged as high Z_{min} events. We have found empirically that the lowest 3 altitude levels of these retrievals – within 2 km of z_{min} - can have higher random scatter in the H_2O and NO_2 profiles. We therefore add an extra error component to these points and flag them as potential bad data.

In order to provide guidance to the POAM data user in screening bad data, the data quality flags for O_3, NO_2 and H_2O has been added to the version 4 archived data. These flag arrays (one per species) give a simple integer value at each altitude for each retrieved profile. The flag values and interpretation are summarized in Table 1:

Flag Value	Meaning
0	Data good
1	High aerosol error
2	High sunspot error
3	High aerosol + high sunspot error
4	High Z_{min}
5	High Z_{min} + high aerosol error
6	High Z_{min} + high sunspot error
7	High Z_{min} + high aerosol error + high sunspot error

Table 1. Description of data quality flags for O_3, NO_2 and H_2O.

Thus, to be very conservative we recommend that the user consult this flag array and eliminate, or use with caution, any point with a non-zero flag value. We would like to emphasize to the user that the extent to which flagged data is eliminated depends greatly on the analysis being performed. When using single POAM profiles in a quantitative analysis, we strongly recommend eliminating, or at least carefully scrutinizing, all screened points. However, when binning the data (e.g., to construct zonal, weekly or monthly means) it is possible to beat down the errors by averaging and the user can be more lax in applying the screens. Of course, the extent to which errors will be reduced by averaging depends upon how Gaussian, or random, the error source is. As we discussed previously, the sunspot errors in particular are not well approximated by Gaussian statistics and the user should be careful in averaging sunspot-flagged data over short time periods (e.g., a few days) since systematic sunspot artifacts can persist in the data over this length of time. For users interested in a more conservative sunspot screen than provided by the flag array, an array called “max_ss” is included in the version 4 data file, corresponding to the maximum POAM sunspot index encountered during each occultation. Any POAM event with a non-zero value in this field has encountered a sunspot of given magnitude somewhere in the instrument field of view during the event.

IV. Summary of Version 3 to Version 4 changes in individual retrieval species

In general, for each species the differences between the version 3 and version 4 retrievals can depend on hemisphere, altitude, season and time. We have tried to summarize the main features of these differences in the following sections.

Ozone, Northern Hemisphere:

At 35 km and above there are no significant changes. From approximately 25-30 km, version 4 ozone is about 0-5% (0.1 – 0.2 ppm) lower than version 3. At 20 km and below the mean differences are generally negligible (less than 0.1 ppm), except at 10 km where version 4 is higher by as much as 15-30% (0.05 - 0.1 ppm) in 2001 and 2002.

Ozone, Southern Hemisphere:

Above 30 km there are not significant changes. At 30 km, version 4 is consistently lower by about 0-5% (~0.1 ppm). From 20- 25 km differences are negligible through 2002, but version 4 is lower by 5-10% (0.2-0.3 ppm) in 2003-2004. At 15 km and below, version 4 is generally higher, primarily in the wintertime. At 15 km and below the enhancement is ~ 0.1 ppm, corresponding to 5-10% (15-20%) at 15(10) km.

Water Vapor, Northern Hemisphere:

The water vapor is significantly less noisy in version 4. In the stratosphere it is also wetter than the version 3 retrievals. From 35-45 km increases are 3-5% (0.2 – 0.4 ppm), with regular seasonal variations such that the maximum difference occurs in summer. Between 25 and 30 km the increase is 5-10% (~ 0.5 ppm), and constant in time. From 15 to 20 km the increase is less than 5 % through 2000, but increases after that, reaching 10-20% (0.5 – 0.7 ppm) by 2004. At 10 km differences with version 3 are also small through 2000, but beginning in 2001 the version 4 retrievals are significantly drier, with a strong seasonal dependence. Differences range from 0-10 % in the winter, to up to 50 % in the summer periods. This is primarily an effect of changes in the version 4 altitude grids, since there is significant altitude sensitivity at the hygropause due to the steep H_2O gradient.

Water Vapor, Southern Hemisphere:

Most of the characteristic differences seen in the Northern Hemisphere water vapor are also present in the Southern Hemisphere. Again, the water vapor is significantly less noisy in version 4. At 35 km and above increases of 3-5% (~ 0.3 ppm) are seen, with the same seasonal dependence. At 30 km the increase is on the order of 5-10% (0.3 – 0.5 ppm). In the 15-25 km region increases of 5-15 % (0.3 – 1.0 pppm) relative to version 3 are seen at all times through 2002, but increase to 20% or more beginning in 2003.
The drier bias at 10 km in Version 4 is smaller than in the Northern Hemisphere, probably due to the lower hygropause altitude. Through 2002 the differences are less than 10-20% (1.0 ppm) but increase to 20-30% (2 - 3 ppm) beginning in 2003.

Nitrogen Dioxide, Northern Hemisphere:

At 35 km and above there is no significant change. NO_2 is about 5-15% (0.2 – 0.5 ppb) lower in version 4 from 27-33 km altitude, with the largest differences occurring in the wintertime. Below 25 km NO_2 is larger, reaching a peak value of about 0.3 ppb larger at about 23 km. The percentage differences vary seasonally due to changes in NO_2

abundance, ranging from 5% or less in the summer to greater than 50% in the winter when NO_2 is extremely low.

Nitrogen Dioxide, Southern Hemisphere:

The Southern Hemisphere exhibits similar systematic differences with version 3 described above for the Northern Hemisphere. Differences are somewhat larger, but seasonally dependent, at 37 km and above. In the summertime differences are negligible, but in the wintertime version 4 tends to be higher by 5-10% (~ 0.1 ppb). The decrease between 25 and 35 km ranges from 0.2 to 0.7 ppb, peaking at 30 km. In relative terms this represents a difference of 5-10% in the summer and up to 50% in the winter. There is a distinct increase in the differences with time at 30 km, from ~ 0.5 ppb in 1998 to 0.7-1.0 ppb by 2004. At 20 km version 4 is higher than version 3 by 0.2 – 0.4 ppb.

Aerosol Extinction at 1 micron, Northern Hemisphere:

One significant change in the version 4 aerosol retrieval is that we are no longer archiving data above 25 km. Because of changes to the instrument altitude retrieval algorithms we have to assume an effective aerosol/Rayleigh extinction ratio to constrain the pointing down to ~ 26 km, so that an independent aerosol retrieval is no longer possible at these altitudes.

Overall the version 4 extinction is higher in the altitude range of 12-23 km. This change is small (< 10%) through 2000, but increased significantly beginning in early 2001. By 2004 the increase was 30-50%, broadly peaking at ~ 17 km. The differences then become smaller in the UT/LS region (10-12 km). There is significant variability in the changes for individual measurements corresponding to large % differences that are difficult to characterize.

Aerosol Extinction at 1 micron, Southern Hemisphere:

The Southern Hemisphere comparisons are generally similar to the Northern Hemisphere. However, the increase with respect to version 3 is evident earlier in time and reach 50-70% at 18 km by 2003. Starting in early 2003, the version 4 extinction difference is larger in the 12-25 km range, approaching 100%. At 10 km, the extinction remains generally higher by 10-30 %, as opposed to the Northern Hemisphere.

References

Lumpe, J. D., R.M. Bevilacqua, K.W. Hoppel, and C.E. Randall, POAM III Retrieval Algorithm and Error Analysis, *J. Geophys. Res.*, *107*(D21), 4575, 10.1029/2002JD002137, 2002.

Randall, C. E., J.D. Lumpe, R.M. Bevilacqua, K.W. Hoppel, E.P. Shettle, D.W. Rusch, L.L. Gordley, K. Kreher, K. Pfeilsticker, H. Boesch, G. Toon, F. Goutail, J.P. Pommereau, Validation of POAM III NO2 measurements, *J. Geophys. Res.*, doi:10.1029/2001JD001520, 2002.