Validation of Ozone profiles retrieved from SAGE III limb scatter measurements

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ABSTRACT
Ozone profiles retrieved from SAGE III limb scatter measurements are compared with correlative measurements made by occultation instruments (SAGE II, SAGE III and HALOE), a limb scatter instrument (OSIRIS) and a series of ozonesondes and lidars, in order to ascertain the accuracy and precision of the SAGE III instrument in limb scatter mode. The measurement relative accuracy is found to be 5-10% from the tropopause to about 45 km whereas the relative precision is found to be less than 10% from 20 to 38 km. The main source of error is height registration uncertainty, which is found to be Gaussian with a standard deviation of about 350 m.

1. INTRODUCTION
The Stratospheric Aerosol and Gas Experiment (SAGE III) instrument on board the METEOR 3 spacecraft was launched in December 2001 to continue NASA’s commitment to monitor ozone and aerosol loading in the upper atmosphere [Mauldin et al., 1998]. As its predecessors (SAM, SAM II, SAGE and SAGE II), SAGE III primary mode of operation is solar occultation. In the past four years, SAGE III has also been used to assess the Limb Scatter (LS) technique which has been selected for future ozone monitoring space instruments such as the Ozone Mapping and Profiler Suite (OMPS) on board the National Polar Orbiting Operational Environment Satellite System (NPOESS) [Flynn et al., in press] and the NPOESS Preparatory Project (NPP) satellites. Over its mission, SAGE III has made approximately 10 000 limb scatter measurements over a wide range of illumination conditions (solar zenith and scattering angles), and over a series of geographical locations ranging from low to high latitudes. Most of SAGE III LS measurements were designed to either coincide (in space and sometimes time) with the measurements of other space instruments such as SAGE II, HALOE, and SAGE III (solar occultation), or were made over a series of ozonesonde and lidar stations. The goal of the present article is to report on the accuracy and precision of ozone profiling achieved by SAGE III in LS mode. This assessment is performed by comparing retrieved ozone profiles with those measured by other instruments. In effect therefore, the reported accuracy/precision estimates are not absolute numbers since they contain other instruments measurement and algorithm errors as well as atmospheric noise.

SAGE III is a 0.5 km vertical resolution grating spectrometer, and its main characteristics are summarized in Section 2. In LS mode, its scan mirror is set to slowly scan the Earth limb at a rate of one spectrum per 0.25 km. The measured radiance spectra are analyzed to retrieve ozone density vertical profiles, as well as NO₂ concentration, multi-wavelength aerosol extinction, cloud height and effective scene albedo. The data analysis and retrieval method have been described by Rault (2005) and are briefly summarized in Section 3, together with the latest algorithm refinements. In Section 4, the two different scenarios used to make LS measurements are presented and the available data are described. The correlation criteria used to ascertain retrieval accuracy and precision are explained in Section 5. SAGE III LS retrieved ozone profiles are then compared with the ones measured with solar occultation instruments in Section 6, ozonesondes and lidars in Section 7, and the Optical Spectrograph and InfraRed Imager System (OSIRIS [Llewellyn et al., 2004]) LS instrument in Section 8. SAGE III LS retrieved ozone profiles are also compared to the ones computed with the NASA Regional Air Quality Modeling System model (RAQMS) in Section 9. To estimate the precision of SAGE III in limb scatter mode, a series of measurements were made over the same geolocations on consecutive orbits, as described in
section 10, where precision is estimated to be on the order of 3%. Several parameters are known to affect the accuracy and precision of limb scatter ozone retrievals, such as atmospheric composition (aerosol, NO$_2$), scene albedo, tangent height registration and inhomogeneities [Loughman et al., 2005]. The final section discusses the sensitivity of ozone retrieval to stratospheric aerosol, NO$_2$, effective scene albedo and tangent height offsets.

2. SAGE III INSTRUMENT

2.1 Instrument characteristics
SAGE III is a grating spectrometer that measures ultraviolet (UV), visible and near infrared (IR) radiances from 280 to 1040 nm at a spectral resolution of 1.3 to 2.8 nm. Its field of view is 0.5 arc minute in elevation, which corresponds to a vertical resolution of 0.5 km, and 4 arc minutes in azimuth when operating in limb scatter mode. Wavelength registration has been found to be very stable and little shift has been observed over the past three years of operation. SAGE III was launched in December 2001 in a sun synchronous orbit (ascending node time of about 9:15 AM local solar time) with a mean altitude of 1020 km and a period of 105 minutes. The SAGE III aperture is mounted in a nadir direction and its line of sight is controlled by a rotating head in azimuth and a scan mirror in elevation. [Mauldin et al., 1998]

2.2 SAGE III in limb scatter mode
The operating mode selected for limb scatter measurement is as follows: integration time of 1/16 second, 16 Hz data acquisition rate, 340 spectral channels available for downlink. Data acquisition is limited to 4-5 minutes per orbit, because of limited on board storage capability and the instrument thermal behavior. The limb is typically scanned from -60 km to 165 km at a rate of 4 arc minutes per second, which corresponds to a scan duration of about 1 minute and a vertical sampling of 0.25 km between consecutive spectra. Each measurement opportunity (hereafter called “event”), therefore comprises 4-5 scans and about 900 spectra per scan. The downlinked spectral channels are selected to primarily focus on the retrieval of ozone, nitrogen dioxide and aerosol. Other channels are included to investigate the molecular oxygen $A$, $B$ and $\gamma$ bands and water vapor.

3. RETRIEVAL ALGORITHM

The retrieval algorithm used to infer ozone profiles from SAGE III limb scatter radiance measurements is described by Rault (2005). SAGE III was specifically designed to operate in occultation mode (bright source over dark background, altitude registration derived from ephemeris), and no provision has been made to mitigate off-axis stray light or precisely measure the instrument pointing direction. SAGE III limb scatter data is therefore characterized by high stray light contamination, poor dark current characterization and poor spacecraft attitude information. A first order model has been developed to attempt to quantify stray light level and dark current and remove their effect from raw data. This first order model is based on the definition of an effective slit function, which is determined solely from high altitude radiance data. Altitude registration is determined using the RSAS method [Janz et al., 1996] and a modified version of the Knee method [Sioris et al., 2003]. The straylight-corrected and altitude-registered data, a sample of which is illustrated in Figs 1a,b, can be observed to contain the absorption signature of several gases such as ozone (Huggins band in UV and Chappuis band in visible), NO$_2$ (between 435 and 450nm) and molecular oxygen. Stratospheric aerosol scattering is also visible in the data, in the form of a radiance increase between 20 and 30km. Two techniques have been implemented to retrieve ozone density vertical profiles. The first one is based on the Triplet method [Flittner et al., 2000] and the second one is based on Multiple Linear Regression (MLR) [Bevington, 1969]. The MLR method was found to be better suited to the analysis of SAGE III data, as the MLR residuals contain information on “unaccounted for” instrument effects (such as residual straylight and dark current), which can then be modeled and removed from the data. Since sensitivity analyses [Loughman et al., 2005] have shown that LS ozone retrieval accuracy is affected by uncertainties on clouds, aerosol loading, surface albedo and NO$_2$, the retrieval algorithm is composed of two parts. In the first one, the cloud height, aerosol extinction vertical profile and the effective surface albedo are estimated using a series of non absorbing channels following the method described by Rault (2004). In the second part, NO$_2$ is first retrieved, using an MLR approach (Rault-2005), and subsequently, ozone vertical profile is retrieved using UV and visible channels. Figure 2 shows typical SAGE III LS products, namely vertical profiles of ozone, NO$_2$ and aerosol extinction. Retrievals are nominally
performed over an altitude range of 10 km (or the cloud height, whichever is higher) to 48 km. In most cases, the triplet and MLR methods yield similar results, within the retrieval uncertainty. A composite ozone profile is constructed using both the Huggins and the two Chappuis retrievals, using the retrieval uncertainties and averaging kernel matrix diagonals as weighting factors.

4. MEASUREMENT SCENARIOS

Since SAGE III was designed to operate in solar and lunar occultation modes only, the instrument duty cycle was anticipated to be relatively low. Consequently, the onboard data storage allocated for the mission is minimal and only allows for a limited number of limb scattering events to be planned between data downlinks, typically one 5-minute event per orbit. Furthermore, limb scatter measurements can only be performed on days when lunar occultations are not possible, which limits limb scatter measurements to about 6-7 days per month. In view of these limitations and to optimize the science return, limb scatter measurements were made in one of two ways:

1) **Measurements within a set of latitude bands:** Each day, a relatively narrow latitude band of ~ 15° is selected and limb scatter measurements are made over a 5 minute period within that band. On each orbit, the latitude band is chosen to encompass the tangent point location of other space instruments, such as SAGE II, SAGE III or HALOE. To simplify instrument operation, the instrument azimuth angle is kept constant, typically 180°, corresponding to the instrument pointing in a rearward direction. This mode of measurement allows one to assess SAGE III LS products accuracy by comparing SAGE III LS retrievals with the measurements made by well characterized instruments.

2) **Measurements over a series of ground stations:** A series of ground stations is selected among the tropical SHADOZ ozonesonde stations network [Thompson et al., 2003] and limb scatter measurements are made each time the station comes in view of the SAGE instrument. The instrument azimuth angles are necessarily adjusted to point the instrument towards the targeted station. Typically, a given station can be seen on two or three consecutive orbits. This mode of measurement allows one to assess SAGE III LS products precision (degree of repeatability) by comparing the retrievals made at the same location over a short period of time (±100 minutes) for a range of solar zenith and scattering angles. When possible, coincident ozonesonde measurements are made at the time of SAGE III overpass to assess the measurement accuracy.

5. ACCURACY AND PRECISION DETERMINATION

In the period between 2002 and 2006, SAGE III has made more than 10000 limb scatter measurements over a wide range of latitudes, solar zenith angles and scattering angles. To ascertain the accuracy and precision of these measurements, a search was made to identify collocated measurements made by other space instruments, ozonesondes and lidars, and a comparison of the retrieved profiles was made on a statistical basis. The collocation criteria used for comparison are as follows:

- latitude separation is less than 3°
- longitude separation is less than 20°
- time separation is less than half a day
- TOMS total ozone difference at the two measurements locations is less than 20 Dobson units. This requirement was imposed to ensure that both measurements belong to the same airmass

Four parameters are used to compare SAGE III LS retrieved profiles with correlated ones, namely (1) mean profiles, (2) mean bias, (3) standard deviation and (4) altitude offset. The mean profiles are constructed on a one km grid as the mean value over the whole ensemble of coincident events. The mean bias is the difference between the two mean profiles. The standard deviation is evaluated as the root mean square with the bias removed. The altitude offset is computed with a stretch and shift algorithm to establish the altitude shift required to obtain the highest correlation between the SAGE III LS retrieved profile $O_3^{SAGE3}(h)$ and the correlated profile $O_3^{correl}(h)$:

$$O_3^{SAGE3}(h) = \text{Norm.}[O_3^{correl}(h) + \Delta h \hat{\partial} O_3^{correl}(h) / \hat{\partial} h]$$  

Equation 1
where \( h \) is the altitude, \( \Delta h \) is the altitude offset and Norm is a constant multiplier.

6. CORRELATION WITH SOLAR OCCULTATION INSTRUMENTS

Figure 3a shows a comparison of SAGE III LS measurements with SAGE II occultation measurements. The measurements were made over a latitude band ranging from 20° to 50° North (Fig. 3b). The top left panel shows the mean (67 profiles), with the NCEP tropopause height depicted as a black horizontal line. The bottom left panel shows the bias between the two mean profiles. This bias is a measure of the retrieval accuracy when compared with SAGE II. It can be observed that the bias is within 5% from the tropopause to 45 km. Below the tropopause, the bias increases to more than 10%, probably due to inhomogeneities within the troposphere. The top right panel shows the standard deviation, which is a measure of the retrieval precision when compared to SAGE II. It can be observed that the standard deviation is less than 10% between 20 and 36 km. Below 20 km, the standard deviation is rapidly increasing mainly due to increased atmospheric variability at the lower stratosphere upper troposphere region. The dotted line represents the composite retrieval 1 \( \sigma \) uncertainty. The lower right panel shows the altitude offset histogram. This is a measure of the height registration error, which can be characterized by a Gaussian curve with an offset of -90m and a FWHM of ±340m.

Figure 4a shows a similar comparison between SAGE III LS and SAGE III occultation retrievals, using 41 profiles. The measurements were made over a narrow latitude band ranging from 30° to 40° south. The mean bias is within 5% from the tropopause to 30km. Above 30 km, the bias increases but remains within 10%. The standard deviation shows the same trend as in the case of SAGE II and the height registration uncertainty is also about the same.

Figure 5 illustrates the comparison between SAGE III LS and HALOE (60 profiles). The mean bias remains within 5% from the tropopause to 45km, while the standard deviation is less than 10% from 20 km to 35 km. The height registration appears to have a null offset and an RMS error of 450m.

To derive absolute values for accuracy and precision for SAGE III LS from these comparisons is not possible, since the mean bias and standard deviation derived in this analysis also depend on the accuracy/precision of the other instruments used to make the comparison and on the natural variability of the atmosphere. The mean bias and standard deviation discussed above are only the upper bounds of SAGE III LS accuracy and precision respectively. To illustrate this point, Fig. 6 shows a comparison of SAGE II retrieved ozone profiles with the ones obtained from various occultation, balloon sondes, and groundbased instruments. The mean bias can be seen to be less than 5% whereas the standard deviation is between 7% and 10% in the altitude range 20-40 km. However, recent inter-comparison campaigns have shown that the SAGE ozone measurements can be estimated to have a precision of 2% or better in the lower stratosphere [Borchi et al., 2004].

7. CORRELATION WITH OZONE SONDES AND LIDARS

Figure 7 shows a comparison of SAGE III LS ozone retrieval with measurements made by a series of ozonesondes spread over both hemispheres (180 profiles, 23 stations). The mean bias between SAGE III LS retrievals and ozonesonde measurements is within 5% from the tropopause to 30 km, with the standard deviation less than 10% between 22 km and 33km. Altitude registration discrepancies have an offset of -350m and a FWHM of ±390m. Figure 8 shows similar results obtained when comparing SAGE III LS ozone profiles with lidar measurements (43 profiles, 4 stations). Table 1 is summary of ozonesondes and lidar measurements used in this work.

8. CORRELATION WITH OSIRIS LIMB SCATTER INSTRUMENT

Figure 9 shows a comparison of SAGE III LS ozone retrieval with OSIRIS ozone profiles (Version 012). The measurements were made over North America and Northern Atlantic ocean between and 30 and 70° North during July 2004 (320 profiles). Mean bias can be seen to be less than 8% from tropopause to 36 km, with standard deviation lower
than 10% between 20 and 36 km. These findings are compatible with the ones obtained by Petelina (2005) who observed OSIRIS biases with other space instruments (POAM III and SAGE III) to be 7% in the altitude range 16-30 km, 10-20% in the altitude range 30-32 km and larger biases at higher altitudes. Altitude registration discrepancies have an offset of -100 m and a FWHM of ±470 m.

9. CORRELATION WITH RAQMS MODEL

Figure 10 shows a comparison of SAGE III LS ozone retrieval with the profiles generated by UW/NASA-LaRC Regional Air Quality Modeling System (RAQMS) for a series of measurements which were made over North America and Northern Atlantic ocean between and 30 and 70° North in July 2004. RAQMS (Pierce et al., 2003) is a multi-scale chemical/dynamical modeling and data assimilation system combining two meteorological forecast models (regional domain nested within a global domain) with a stratospheric-tropospheric chemical prediction scheme. It simulates processes involving the long-range transport of trace constituents and resolves atmospheric structure on spatial scales as low as 5 km in horizontal and 200-400 m in vertical. Stratospheric profiles from SAGE and HALOE, together with total ozone column measurements from TOMS, are presently assimilated in the model. Comparing SAGE III LS products with RAQMS computed profiles therefore in effect allows one to compare SAGE III LS retrievals with a combination of occultation instruments, with the model providing information on chemical transport between occultation and limb scatter measurement geolocations. In the present work, RAQMS is used to compute ozone profiles at the exact location and time of SAGE III LS measurements (593 profiles). The results depicted on Fig. 10 show a mean bias between SAGE III LS and RAQMS of less than 7% between 20 km and 38 km, with standard deviation less than 10% between 23 and 37 km. The larger mean bias values at lower altitudes are probably due to discrepancies in stratospheric aerosol distributions. Altitude registration shows no offset and a FWHM of ±350 m.

10. PRECISION AND SELF CONSISTENCY EVALUATION FROM JUNE 28, 2004 MEASUREMENT OVER LA REUNION

Figure 11 illustrates the limb scatter experiment which was conducted on June 28, 2004 over La Reunion island off the coast of Madagascar. During the first orbit, the spacecraft is passing to the east of La Reunion and, at the station, the solar zenith angle is 75-77° and the scattering angle is 165-168°. In the second orbit, the spacecraft flies almost overhead and, at the station, the solar zenith angle is 55-60° and the scattering angle is 122-127°. Finally, in the third orbit, the spacecraft is passing to the west of La Reunion and, at the station, the solar zenith angle is 44-51° and the scattering angle is 98-100°. TOMS data is superimposed on Fig. 11 to highlight the total ozone distribution around La Reunion on that day. Figure 12 shows the SAGE III LS ozone profiles for each of the four scans and compares them with the profile measured by the ozonesonde, which was launched at La Reunion in between the first and the second orbit. A good comparison can be observed from orbit to orbit, which underscores the self consistency of the retrievals in spite of the relatively large range of solar zenith and scattering angles. That self consistency can further be seen in Fig. 13 which shows the standard deviation (with respect to the mean profile for each scan) for each of the four scans. The standard deviation is close to 3% from 20 km to 40 km. This set of measurements compares SAGE III LS with itself, with only the actual location of the tangent point changing from one orbit to the next. This last effect is difficult to evaluate, but may not be negligible as indicated by the gradients in total ozone observed by TOMS. Using the stretch and shift method described above, the altitude uncertainty from orbit to orbit was found to have a mean of 0 m and a standard deviation of 150 m.

11. DISCUSSION

The accuracy and precision of SAGE III ozone limb scatter products depend on several factors, some of which are instrument related (straylight, dark current) and some of which are due to the unknown state of the atmosphere and surface conditions, such as:

- Aerosol vertical distribution
- NO₂ density profile
- Scene reflectance
- Inhomogeneity of underlying surface
- Inhomogeneity of ozone along satellite track

Additionally, uncertainties in tangent height registration induce errors in ozone accuracy (constant height offset leads to increased bias) and precision (algorithm deficiency and radiance/atmosphere noise increases the standard deviation). The first three parameters are retrieved prior to the ozone retrieval in the standard SAGE III data analysis algorithm, but the accuracy of their retrieval is difficult to ascertain. The mean effect of these three parameters on ozone profiling can however be estimated thru a sensitivity analysis performed over a large ensemble of SAGE III Limb Scatter data sets. Figure 14 shows that a change of surface reflectance from 0.05 to 0.5 would lead to an ozone density increase of about 4% from the tropopause to 30 km. Figure 15 shows that ignoring aerosol contribution (aerosol extinction=0) would produce a negative ozone density bias of up to 7% in the lower stratosphere. Figure 16 shows that neglecting NO₂ contribution (NO₂ density = 0) would lead to an ozone error of less than 3% from 15 to 45 km. The effect of inhomogeneity on ozone retrieval is a more complex problem and cannot readily be evaluated from SAGE III limb scatter data, but will to be addressed when dealing with NPOESS/OMPS data. Scene inhomogeneity (due to clouds, land cover, land/ocean transition) would affect the measurement precision by several percents (see Fig.14). Along track inhomogeneity could be particularly severe in regions of large horizontal ozone gradients, such as near polar vortices and within the troposphere. The effect of tangent height registration uncertainty on ozone retrieval can be estimated from Figure 17 which shows the ozone profiling sensitivity to a 1 km tangent height shift. Since SAGE III height registration error is estimated to be 350m, tangent height registration is estimated to affect ozone precision by 3-5%.

12. CONCLUSION

In this paper, the relative accuracy of SAGE III in limb scatter mode is estimated to be 5-10% for altitudes ranging from tropopause to 45km, while the relative precision is estimated to be less than 10% from 20km to 38km. Height registration is identified as a primary source of uncertainty. This analysis shows the potential of SAGE III to monitor ozone vertical profiles in LS mode, in spite of serious instrument shortcomings, such as high straylight contamination, lack of dark current measurement and poor instrument pointing accuracy. The good comparison between SAGE III LS retrieved profiles with correlated data attests to the overall quality of the retrieved ozone profiles and therefore to the adequacy of the approach used to (1) clear instrument effects from raw radiances data, (2) retrieve ozone information from limb scatter spectra and (3) infer height registration information from radiances profiles. The lessons learnt with the SAGE III LS data set are presently being applied to prepare the OMPS instrument, on which the scientific community will rely for future ozone profile monitoring from space. In view of the good quality of SAGE III LS products, this data set will be used in further studies to tackle remaining issues such as the effect of scene inhomogeneity and height registration accuracy.

As the scientific community gradually transitions from occultation instruments (SAGE, HALogen Occultation Experiment (HALOE), Polar Ozone and Aerosol Measurement (POAM) to limb scatter instruments (SCIAMACHY on ENVISAT, OSIRIS on Odin, OMPS on NPP and NPOESS) to perform ozone profiling from space, SAGE III dual mode capabilities can be utilized to evaluate both techniques simultaneously on the same space platform. The limb scatter technique has several advantages over solar/lunar occultations, among which, larger geographical coverage and longer duty cycle (can be done over the whole sunlit portion of the orbit as opposed to a few minutes before and after sun/moon rises and sets). However, the limb scatter technique has yet to be proven to be sufficiently accurate to rival and replace occultation techniques in future monitoring of global ozone trend analyses. Present efforts in the validation of the limb scatter instruments, together with the advent of new limb scatter instruments, such as OMPS on NPP and NPOESS will help in better defining the strength and future of this technique.

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REFERENCES


Table 1 Summary of ozonesondes and lidar measurements
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Figure 1a. Typical SAGE III Limb Scatter radiance spectral data

Figure 1b. Typical SAGE III Limb Scatter radiance profile
Figure 2. SAGE III Limb Scatter retrievals. Ozone, NO₂, aerosol extinction.

Figure 3a. Comparison of SAGE III LS retrieved ozone profiles with SAGE II products. (SAGE III LS solar Zenith angles from 40° to 81°, scattering angles from 36° to 140°, surface albedo from 0 to 0.4)
Figure 3b. Geolocations for comparison of SAGE III LS and SAGE II products

Figure 4. Comparison of SAGE III LS retrieved ozone profiles with SAGE III solar occultation products (SAGE III LS solar Zenith angles from 34° to 43°, scattering angles from 92° to 108°)
Figure 5a. Comparison of SAGE III LS retrieved ozone profiles with HALOE products (SAGE III LS solar Zenith angles from 18° to 82°, scattering angles from 36° to 172°)

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Figure 6. SAGE II ozone products compared with other occultation instrument products and ozonesondes.

Figure 7. Comparison of SAGE III LS retrieved ozone profiles with ozone sonde measurements. (SAGE III LS solar Zenith angles from 28° to 88°, scattering angles from 35° to 150°)
Figure 8. Comparison of SAGE III LS retrieved ozone profiles with lidar measurements. (SAGE III LS solar Zenith angles from 36° to 87°, scattering angles from 44° to 102°)
Figure 9a. Comparison of SAGE III LS retrieved ozone profiles with OSIRIS products. (Zenith angles = 40-60° (SAGE), 65-80° (OSIRIS), scattering angles = 55-70° (SAGE), 60-110° (OSIRIS), Surface albedo = 0.0 – 0.5)

Figure 9b. Geolocations for comparison of SAGE III LS and OSIRIS products
Figure 10a. Comparison of SAGE III LS retrieved ozone profiles with RAQMS model. (SAGE III LS solar Zenith angles from 40° to 60°, scattering angles from 56° to 86°)

Figure 10b. Geolocations for comparison of SAGE III LS and RAQMS model products
Figure 11. Tangent points geolocation for SAGE III measurements over LaReunion overplotted over TOMS total ozone map. Red, green and blue broken lines correspond to successive orbits, 105 minutes apart.

Figure 12. Ozone vertical profiles retrieved from SAGE III LS radiance on consecutive orbits, compared with ozonesonde measurements.
Figure 13. June 28, 2004 measurements. Standard deviation (around mean for each scan)

Figure 14. Effect of scene albedo uncertainty on ozone retrieval
Figure 15. Effect of stratospheric aerosol on ozone retrieval

Figure 16. Effect of NO$_2$ on ozone retrieval

Figure 17. Effect of 1km height registration offset on ozone retrieval