The retrieval of ozone profiles from limb scatter measurements: Results from the Shuttle Ozone Limb Sounding Experiment

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Abstract. Two instruments were flown on shuttle flight STS-87 to test a new technique for inferring the ozone vertical profile using measurements of scattered sunlight from the Earth's limb. The instruments were an ultraviolet imaging spectrometer designed to measure ozone between 30 and 50 km, and a multi-filter imaging photometer that uses 600 nm radiances to measure ozone between 15 km and 35 km. Two orbits of limb data were obtained on December 2, 1997. For the scans analyzed the ozone profile was measured from 15 km to 50 km with approximately 3 km vertical resolution. Comparisons with a profile from an ozonesonde launched from Ascension Island showed agreement mostly within ±5%. The tropopause at 15 km was clearly detected.

Introduction

Fifteen years ago most models predicted that the largest changes in ozone as a result of the introduction of chloro-fluorocarbons (CFCs) into the atmosphere would be observed in the upper stratosphere - in the 40 to 45 km region [*WMO*, 1982]. The discovery of the ozone hole demonstrated that very large changes were occurring in the lower stratosphere in the Antarctic as a result of heterogeneous chemistry. *Stolarski et al.* [1991] showed that significant changes in total column ozone were also being observed at mid- to high latitudes in the northern hemisphere. Many observations summarized in a recent report on ozone profiles [*SPARC*, 1998] show that much of this change in total column ozone is occurring in the 15 to 20 km region.

The backscatter ultraviolet (BUV) instruments flown by NASA [*Fleig et al.*, 1990] and NOAA [*Planet et al.*, 1994] are well designed to measure ozone change in the upper stratosphere. These instruments detect the ozone change in altitudes below 25 km but offer little information about the altitude at which the change is occurring. Limb occultation instruments like the Stratospheric Aerosol and Gas Experiment (SAGE II) [*Mauldin et al.*, 1985, *Cunnold et al.*, 1989], and the Halogen Occultation Experiment (HALOE) [*Russell et al.*, 1993], are capable of retrieving ozone profiles from the troposphere (if there are no clouds) to near 60 km, with approximately 1 km vertical resolution.

The sampling limitations of occultation instruments increase the uncertainty of the ozone trends derived for the lower stratosphere, while the poor information content of the backscatter ultraviolet instruments severely limits their usefulness for determining these trends. What is needed is an instrument with vertical resolution similar to that of an occultation instrument but with coverage similar to that of a

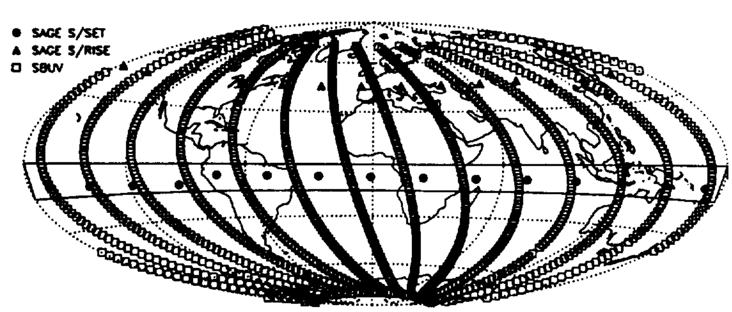

Figure 1 The sampling possible from an occultation instrument (sampling similar to SAGE) compared with the sampling possible from a limb scatter instrument (sampling similar to SBUV).

backscatter ultraviolet instrument. The measurement of limb scattered sunlight offers the possibility of combining the best features of these two measurement approaches. Figure 1 shows the sampling possible from an occultation measurement (using SAGE II as an example) compared with that possible from a limb scatter instrument (using SBUV as an example of an instrument with similar coverage). *Flittner et al.* [this issue] have outlined the theoretical basis for a limb scatter ozone retrieval. In this paper we present the results of applying this retrieval to data taken by demonstration instruments flown on the space shuttle in December of 1997.

The Instruments: SOLSE and LORE

Two instruments were built to test the concept of using limb scattering to measure an ozone profile, the Shuttle Ozone Limb Sounding Experiment (SOLSE) and the Limb Ozone Retrieval Experiment (LORE). SOLSE is a UV imaging spectrometer, while LORE is a filter photometer with a Chappuis band channel at 600 nm. As shown by *Flittner et al.* [this issue] the large ozone cross sections available in the ultraviolet are needed to give good sensitivity to ozone in the upper stratosphere where ozone amounts are small. But in the lower stratosphere Rayleigh scattering, which varies as λ^{-4}, limits limb penetration in the ultraviolet, so that ozone can be reliably measured only down to about the 30 km level. In order to measure ozone at lower altitudes it is necessary to use wavelengths near 600 nm, where Rayleigh scattering is less by about a factor of four.

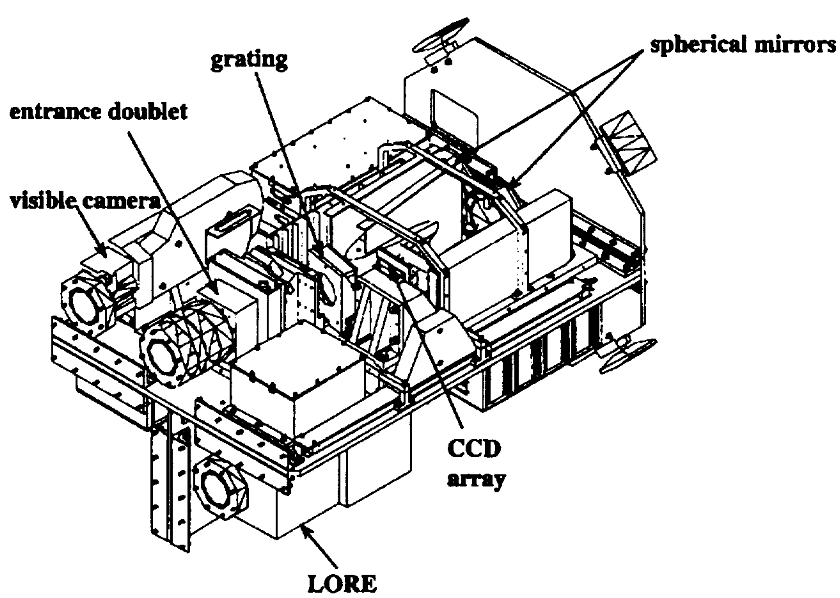

Figure 2 Optical layout of SOLSE (with LORE).

SOLSE is a Czerny-Turner imaging spectrometer designed to produce a high quality image of the limb of the Earth while minimizing internal scattered light (Figure 2). The purpose of SOLSE is to measure ozone in the 30 to 50 km region. The spectrometer covers the range 275 nm to 360 nm with 0.22 nm resolution. The resolution of the vertical image is about 1 km. The detector on SOLSE is a 1024 by 1024 backthinned, UV enhanced CCD array manufactured by SITE. A shutter was used to control the exposure of each frame. Internal scattering is a concern because there is more than 2 orders of magnitude dynamic range in the image from the short-wavelength high-altitude part of the image to the long-wavelength low-altitude part.

LORE is a multi-filter imaging photometer with a linear diode array detector. The purpose of LORE is to measure ozone in the 15 to 35 km region. The filters used were ion-assisted deposition interference filters made by Barr at wavelengths of 345, 525, 600, 675, and 1000 nm, each with about 4 nm bandpass and negligible out of band response. The 600 nm channel is the ozone sensitive channel, while the 525 and 675 nm channels are used for background aerosol subtraction. The 1000 nm channel is used to detect aerosols. The 345 nm channel gives overlap with SOLSE and is used to determine the pointing. LORE is a successor instrument to the Rayleigh Scattering Attitude Sensor (RSAS) [*Janz et al.*, 1996a] which was flown on STS-72 in January of 1996. RSAS showed that the rapid fall-off of 350 nm Rayleigh scattering with altitude could be used to determine pointing to within at least 0.05°. This principle was used to set the pointing of both SOLSE and LORE.

Prior to the shuttle flight, both the SOLSE and LORE instruments underwent extensive characterization and calibration measurements. Spatial point spread functions were measured on both instruments using a back-illuminated slit which was imaged onto the detector. The spectral bandpass and wavelength calibration for SOLSE was measured using line sources while the bandpass of the LORE filters was measured at Research Support Instruments. The results of these measurements are summarized in Table 1. The SOLSE bandpass was found to be temperature dependent due to defocusing of the beam from structural expansion/contraction. The LORE bandpass varied by filter.

Table 1: Spatial and spectral performance of instruments.

Instrument	spatial (FWHM)	spectral (FWHM)
SOLSE	3 pixels (1.2 km at limb)	0.22 - 0.32 nm
LORE	2 pixels (0.5 km at limb)	3.8 - 4.6 nm

Stray light response was measured in the SOLSE instrument by looking at pixel responses above and below the slit image on the CCD array. The magnitude of this signal was typically 1.5% of the in-field signal when illuminated with a flat field source. This magnitude is consistent with the combination of residual signal in the tail of the point spread response (optical blurring) plus a volume scatter term from the optical surfaces. Out-of-field response was measured by scanning a source outside the 2.3° FOV and was found to be negligible. Similar measurements were performed with the LORE instrument yielding a 1% internally scattered light response and negligible out-of-field response.

Both instruments were absolutely calibrated via an integrating sphere and FEL transfer method [*Janz*, 1996b, *Heath*, 1993] to an accuracy of about 3%. The integrating sphere has been successfully used on other atmospheric sensors such as TOMS, GOME, SBUV, and SCIAMACHY. The radiometric calibration was repeated after flight and showed only minor changes in the overall sensitivity of both instruments.

Results from STS-87: Instrument Performance

The SOLSE and LORE instruments were flown as a single payload on shuttle flight STS-87, which was launched on November 19, 1997 and lasted 16 days. The SOLSE/LORE mission was a Hitchhiker Jr. class payload in which the instruments are mounted in a sealed GetAway Special can with a door that opens for observation and with limited data transmitted to the ground. Latitude coverage was limited to ±28° because of the low orbital inclination of this mission. Two orbits of Earth-viewing data were taken, on November 20th and November 27th, and then two orbits of limb-viewing data were taken on December 2nd. The Earth-view data (nadir looking instead of limb looking) were taken in order to compare with data taken by the Total Ozone Mapping Spectrometer (TOMS) on Earth Probe and with spectra from the Global Ozone Monitoring Experiment (GOME) on ERS-2. These comparisons verified that the calibration of SOLSE was consistent with both TOMS and GOME to within 10%.

When the two orbits of limb-view data were analyzed, two problem areas were found. The most serious problem was an error in the exposure setting software that caused most of the data in the troposphere and lower stratosphere to be overexposed. This had little effect on the SOLSE data since that instrument is designed to measure ozone above 30 km, but it limited the usefulness of the LORE data. Out of 133 limb scans taken over the two orbits, only 8 were well exposed in the entire 10 km to 40 km height range.

The second problem was with scattering and reflections within the instruments. During flight the hitchhiker bulkhead window used for the LORE instrument retro-reflected a significant amount of in-band signal from either the detector surface or the filter surface back into the instrument, thus elevating the response by as much as 5-6% at 525 nm, which can represent a large percentage error relative to the limb radiance. This was due to an incorrect antireflection coating on the window. Fortunately this retro-reflection problem mainly affected the high altitude part of the LORE signal. A post-flight characterization allowed us to correct the LORE images, but the profile analysis shown below was cut off at 30 km in order to minimize possible error from this source.

Scattered light was, as expected, a problem with the short wavelength high altitude SOLSE data because of the large dynamic range involved. The scattered light levels observed in-flight closely matched the pre-flight characterization, but residual errors in the scattered light correction were significant at wavelengths shorter than 300 nm because of the low absolute intensity at these wavelengths. This limited the maximum altitude for which ozone could be retrieved from SOLSE data to about 50 km.

Result from STS-87: Data Analysis

The algorithm described by *Flittner et al.* [this issue] was applied to scans measured by SOLSE and LORE on December 2nd, 1997. The scans selected for analysis were ones taken on the second orbit near the equator for which the LORE scans were well exposed in the troposphere. These scans were also closest to Ascension Island, where a balloon sonde was flown to validate the retrieved ozone profile.

Figure 3(a) shows the radiance profiles for two wavelengths measured by SOLSE (322 nm and 345 nm channels) and one LORE wavelength (600 nm). Note the increasing contribution of internally scattered light in LORE in the 600 nm radiance between 40 and 50 km. Also note the reduced radiance near 20 km caused by ozone absorption. Because of the differences between the two instruments, profiles were retrieved for each separately rather than in a single

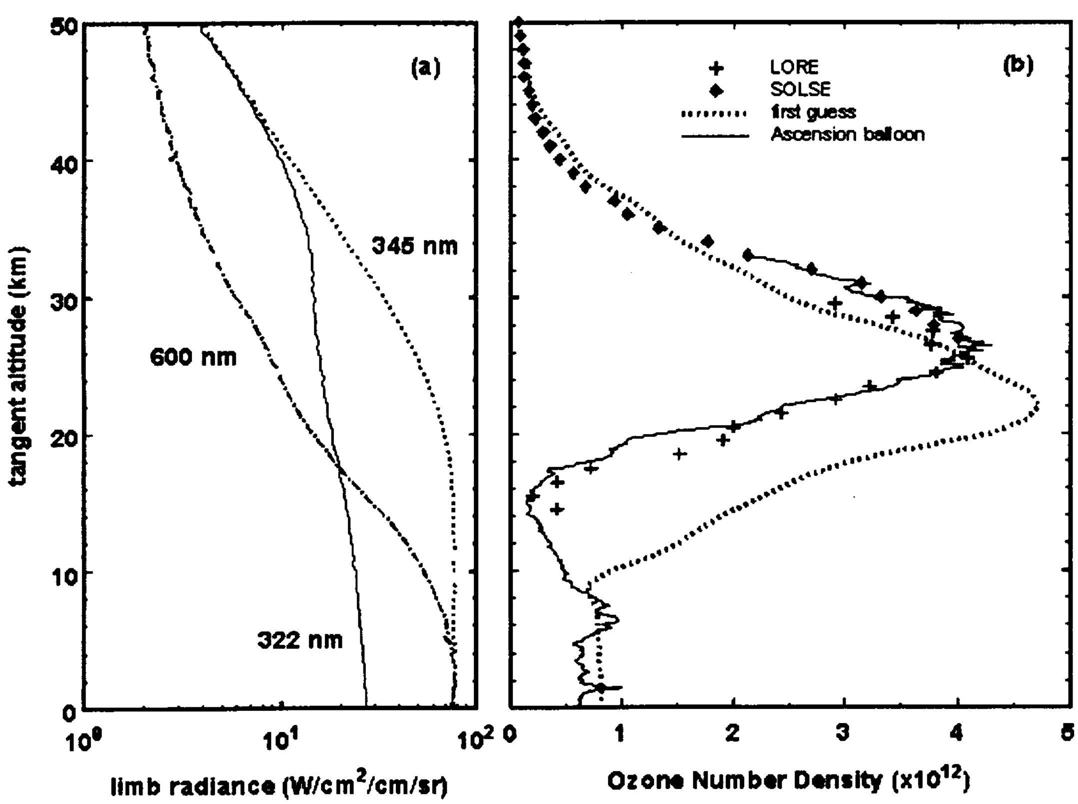

Figure 3 Radiance versus altitude measured by SOLSE (322 and 345 nm) and by LORE (600 nm) is shown in (a), while the retrieved ozone profiles are shown in (b) compared with a balloon-sonde profile measured at Ascension Island.

integrated retrieval as would be done for an operational instrument.

The pointing for each instrument was determined using the 345 nm channel radiances. This technique for determining pointing is based on the fact that at 345 nm the transition from optically thin to optically thick produces a "knee" near 20 km (Fig. 3a) that is insensitive to tropospheric variations. This knee can in principle be located to within 0.01° [*Janz et al.*, 1996a]. When pointing derived using 345 nm was compared with pointing derived from the shuttle attitude sensors, the standard deviation of the agreement translated into ±0.05°, or about ±0.8 km at the limb tangent point.

The SOLSE profile shown in Fig. 3(b) was derived using the Rodgers optimal estimation technique and the algorithm described by *Flittner et al.* [this issue]. Eleven discrete wavelength bands were used: 300, 310, 318, 320, 322, 325, 329, 333, 339, 345, and 355 nm. As the first step in the retrieval, each wavelength was normalized at 45.5 km in order to minimize calibration dependence and reduce the effect of light reflected from clouds and the surface. The covariance matrix for instrument uncertainty was diagonal, set at a constant 1%. The profile retrieval was cut off when the limb optical depth exceeded 1.5, near 27 km for SOLSE. Approximately 3 km vertical resolution was achieved for this profile retrieval.

The LORE retrieval was similar, but used only three wavelength: 525, 600, and 675 nm. The 600 nm channel provides the ozone sensitivity while the 525 and 675 nm channels subtract the effect of aerosols that is linear with wavelength. The optical depth cutoff for LORE was at about 15 km. The upper altitude limit for LORE, 30 km, was imposed to avoid the problems with instrumental scattered light discussed earlier.

In each case a mid latitude ozone profile was used as the first guess (dotted curve in Fig. 3b), even though a low latitude profile would have been appropriate. Our purpose was to clearly demonstrate the independence of the limb algorithm from the assumed á priori profile. (The same profile was used for both the á priori and the first guess.)

In order to validate the limb ozone profile retrieval, electrochemical concentration cell (ECC) ozonesondes [*Komhyr et al.,* 1995] were launched from Ascension Island (7.9°S, 14.4°W) and from La Réunion Island (21.2°S, 55.5°E). Unfortunately LORE performance was not good during the La Réunion Island overpass. The LORE scans used in Fig. 3 were taken at

2°N, 15°W, about 1100 km north of Ascension Island. Despite the lack of a close overpass, the agreement between the balloon profile and the limb retrievals is good. Most importantly, the LORE retrieval appears to have correctly detected the tropopause. The LORE profile near 30 km is lower than either the SOLSE or the ECC profile by about 15%, most likely due to residual scattering error in the LORE high altitude radiances. Otherwise agreement is usually within about 5%, better than would be expected from the uncertainty in pointing and in the radiances (Table 1 in *Flittner et al.*, [this issue]).

Conclusions

Results from the SOLSE/LORE experiment on STS-87 appear to show that limb scattering is a viable technique for monitoring the vertical distribution of ozone. Chappuis band wavelengths are necessary to measure ozone in the lower stratosphere and upper troposphere, while wavelengths in the ultraviolet give the best sensitivity in the upper stratosphere. For the equatorial scans analyzed the profile was measured from 15 km to 50 km with approximately 3 km vertical resolution. The tropopause at 15 km was clearly detected. Because of the large dynamic range involved, an instrument designed to measure the full profile must have very low internal scattering and should have a signal-to-noise ratio approaching 1000 to 1. The technique of determining pointing using the 345 nm channel resulted in pointing accuracy of about 0.8 km. This is just barely adequate for the limb scatter retrieval (though the technique may be capable of 0.5 km accuracy). A more accurate on-board attitude sensor would be very desirable.

The STS-87 results constitute a limited validation of the limb scattering approach to ozone profile monitoring. More extensive measurements over a wide range of latitudes is needed to fully validate the approach. A second flight of the SOLSE/LORE experiment is planned as part of the TAS-3 Hitchhiker bridge, possibly in 2001. For this flight the SOLSE spectrometer will be configured to cover the 600 - 950 nm range in order to better understand the capabilities of this technique in the lower stratosphere and upper troposphere. Finally, limb scattering data from the Stratospheric Aerosol and Gas Experiment III (SAGE III) should be available for analysis in late 2000 or early 2001.

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