Validation of ACE-FTS stratospheric ozone profiles against Odin/OSIRIS measurements

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[1] Stratospheric ozone profiles measured by the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) have been extensively compared with the coincident ozone profiles measured by the Optical Spectrograph and InfraRed Imager System (OSIRIS) on Odin. All coincidences took place between January 31 and August 5, 2004, with the majority in the Northern Hemisphere. ACE-OSIRIS statistical comparisons were performed in the altitude range of 16–32 km where OSIRIS ozone data are in a good agreement, 5–7%, with another satellite and ground-based instruments. At altitudes 3–5 km above and below the ozone peak, ACE-FTS and OSIRIS profiles agree to within ~4–7%, while in the vicinity of the peak the ACE-FTS profiles are systematically lower than OSIRIS profiles by about 10%. This result is consistent for all latitudes between 30°S and 82°N. **Citation:** Petelina, S. V., E. J. Llewellyn, K. A. Walker, D. A. Degenstein, C. D. Boone, P. F. Bernath, C. S. Haley, C. von Savigny, N. D. Lloyd, and R. L. Gattinger (2005), Validation of ACE-FTS stratospheric ozone profiles against Odin/OSIRIS measurements, *Geophys. Res. Lett.*, *32*, L15S06, doi:10.1029/2005GL022377.

1. Introduction

[2] The Atmospheric Chemistry Experiment (ACE) is a recent Canadian satellite mission, launched 12 August 2003, that uses solar occultation to measure the vertical profiles of atmospheric pressure, temperature, aerosols, and many trace gases [*Bernath et al.*, 2005]. A Michelson Fourier Transform Spectrometer (FTS) that operates in the infrared is the primary instrument on ACE. It measures atmospheric temperature, pressure, and extinction profiles, as well as the volume mixing ratios of such trace molecules as H_2O, O_3, N_2O, CO, CH_4, NO, NO_2, HNO_3, HF, HCl, N_2O_5, $ClONO_2$, CCl_2F_2, CCl_3F, COF_2, CHF_2Cl, HDO, and SF_6. One of the main goals of ACE is to study arctic ozone and improve our understanding of the chemical and dynamical processes that control the distribution of atmospheric ozone. The ACE latitudinal coverage ranges from 85°N to 85°S with the majority of occultations occurring near the polar regions, which is advantageous for the study of high latitude ozone chemistry.

[3] The purpose of this work is validation of the first ozone retrievals from the Fourier Transform Spectrometer on ACE (ACE-FTS) through a statistical comparison of these stratospheric ozone profiles with coincident ozone profiles measured by the Optical Spectrograph and Infrared Imager System (OSIRIS) on the Odin satellite. The comparisons are made over the latitude range from about 30°S to 82°N between January and August, 2004. OSIRIS, launched on February 20, 2001, has a proven record of ozone profile measurements through comparisons with other satellite and ozonesonde data [*Petelina et al.*, 2004a, 2004b]. The OSIRIS heritage is beneficial for understanding the recently launched ACE-FTS instrument.

2. Instrumentation

2.1. ACE

[4] ACE is in a high inclination, 74°, circular orbit that provides coverage in the tropical, mid-latitude, and polar regions. The high resolution (0.02 cm^{-1}) infrared Fourier Transform Spectrometer, ACE-FTS, operates in the spectral range from 2 to 13 microns (750–4400 cm^{-1}) and measures the infrared absorption signals during sunrise and sunset. Its field of view is 1.25 mrad, about 4 km, and a vertical sampling is also about 4 km from the cloud tops up to 150 km. This instrument is referred throughout as ACE in the future.

[5] The ACE level 1 data – spectrally calibrated transmittances – are generated with software provided by ABB-Bomem, the instrument contractor. Version 1 of the ACE Level 2 data – atmospheric temperature and pressure, and height profiles of volume mixing ratios of different trace gases – are calculated at the University of Waterloo with the global fit approach of *Carlotti* [1988]. While the original ACE measurements are made with a vertical resolution of about 4 km, the Level 2 data are interpolated on to a 1 km vertical grid.

[6] As the Odin/OSIRIS stratospheric ozone profiles are validated over the altitude range from 16 km to 32 km [*Petelina et al.*, 2004a, 2004b], ACE ozone retrievals outside this height range are omitted from this paper. In the current ACE Level 2 retrieval algorithm, the CO_2 volume mixing ratio is fixed, the pressure and temperature profiles are retrieved from the Level 1 data with the tangent height calculated from hydrostatic equilibrium. The a priori temperature and pressure profiles are a combination of the Canadian operational weather forecast model (GEM) below 30 km and MSIS 2000 atmospheric model above 30 km

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Table 1. Number of Coincidences, Latitude Range, Mean Profile Difference and Standard Deviations (STD) for the OSIRIS and SAGE III Monthly Coincident Ozone Profiles

Month				Mean Profile Diff., %				STD of Profile Diff			
2004	# Coinc	Min. Lat., °	Max. Lat., °	22 km	24 km	26 km	28 km	22 km	24 km	26 km	28 km
Feb	83	48 S	33 S	−1.3	0.7	2.1	0.3	6.8	5.0	5.4	6.2
Mar	22	68 N	81 N	3.0	3.9	−2.2	−5.2	13.7	7.0	4.1	5.4
Apr	85	55 N	72 N	4.0	0.3	−3.5	−9.4	6.4	6.2	10.9	13.4
Jul	54	47 N	56 N	−5.4	0.5	−5.8	−6.4	7.8	9.2	11.6	9.1
Aug	32	50 N	59 N	−4.1	−2.3	−3.3	−4.8	7.3	12.8	9.2	8.1

[*Picone et al.*, 2002]. Further details on the ACE Level 2 retrievals are provided by *Bernath et al.* [2005].

2.2. OSIRIS on Odin

[7] The Odin satellite is a joint Sweden-Canada-France-Finland mission. It is in a sun-synchronous, near-terminator orbit with latitudinal coverage in the orbit plane from 82.2°N to 82.2°S [*Murtagh et al.*, 2002]. In the basic aeronomy mode, Odin scans the Earth limb from 6 to 60 km with a vertical speed of 0.75 km per second. OSIRIS measures the limb-scattered solar radiance in the spectral range 280–810 nm with ~1 nm resolution [*Llewellyn et al.*, 2004]. The OSIRIS vertical resolution of 1 km corresponds to ~250 km horizontal sampling, for ACE the horizontal sampling is ~500 km. During most of the year, OSIRIS provides approximately 30 ozone profiles per orbit over the sunlit hemisphere; this number increases to nearly 60 profiles twice a year during orbital equinox periods.

[8] Ozone number density profiles, version 1.2, are retrieved from the OSIRIS limb radiance spectra on a 2 km vertical grid that covers altitudes from 10 to 48 km. The retrieval algorithm is based on the inversion technique of *Flittner et al.* [2000] and *McPeters et al.* [2000] and has been adapted to OSIRIS by *von Savigny et al.* [2003]. The algorithm uses limb radiance profiles at three wavelengths, two of these are in the wings of the Chappuis absorption band and the third is at the center. The line of sight limb radiances are normalized by measurements at a reference tangent height of 50 km and combined into a Chappuis retrieval vector that serves as input for a non-linear optimal estimation (OE) algorithm [*Rogers*, 1976]. A pseudo-spherical multiple scattering radiative transfer model LIMBTRAN [*Griffioen and Oikarinen*, 2000] is employed as the OE forward model.

[9] OSIRIS stratospheric ozone profiles have been statistically compared on a monthly basis with coincident ozonesonde, Polar Ozone and Aerosol Measurement (POAM) [*Glaccium et al.*, 1996; *Lucke et al.*, 1999], and Stratospheric Aerosol and Gas Experiment (SAGE) [*McCormick et al.*, 1989] measurements. The results of these comparisons have been reported by *Petelina et al.* [2004a, 2004b]. Briefly, the agreement between all instruments in the altitude range of 16–32 km was within 5–7%. Below 16 km, OSIRIS ozone profiles were sometimes affected by high-altitude tropospheric clouds. Between 32 km and 48 km, OSIRIS ozone densities were systematically lower, by up to 20%, than those measured by POAM III, SAGE II, and SAGE III where the cause is most likely instrumental. A small amount of out of field radiation scattered by the OSIRIS baffling is always recorded by the instrument. At high altitudes, where both the limb radiances and the relative ozone absorption signature became smaller, this unwanted signal may impact the retrievals. As this issue is still under investigation, we restrict the ACE and OSIRIS statistical comparisons to the altitude range 16–32 km.

[10] Since OSIRIS makes the ozone measurements in the limb over the sunlit portion of the Earth, the range of comparisons is much greater than is possible from other solar occultation experiments alone. As shown in Section 3, all OSIRIS-ACE coincidences occur between January 31 and August 5, 2004. Consequently, the quality of the OSIRIS ozone retrievals during this time period is of a particular importance. Table 1 presents the statistical comparison of OSIRIS and SAGE III coincident profiles on a monthly basis for approximately the same time period in 2004 as OSIRIS-ACE coincidences. Mean profile differences and their standard deviations in Table 1 are given at four altitudes, 22, 24, 26, and 28 km, in the vicinity of the ozone peak. Apparently, both sets of measurements agree within about 6% except around 28 km in April when the agreement is within 9.4%.

3. Results and Discussion

[11] For the OSIRIS-ACE comparisons we adopted the same coincidence criteria as those in previous OSIRIS

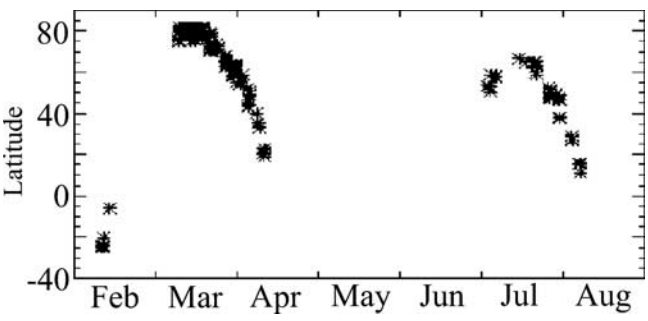

Figure 1. Locations of the ACE-OSIRIS coincidences between January 31 and August 5, 2004.

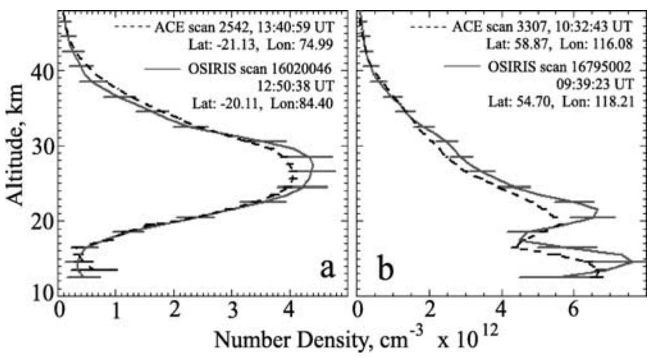

Figure 2. Typical examples of the smooth (a) and structured (b) individual ACE-OSIRIS coincident profiles.

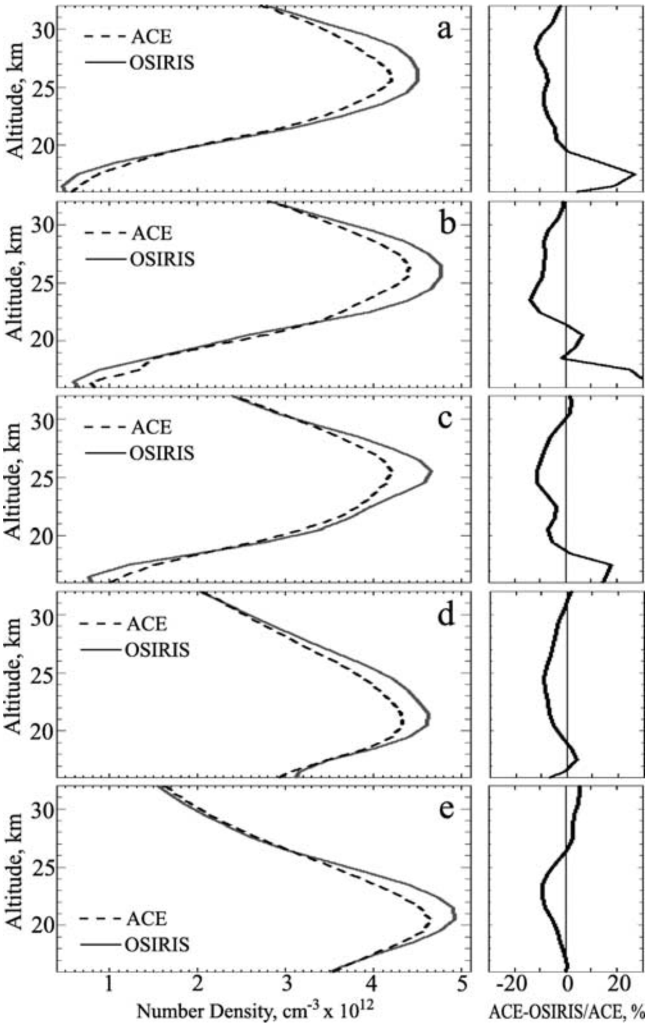

Figure 3. Panels (a)–(e) on the left side: ACE and OSIRIS zonal mean coincident ozone profiles in the latitude ranges of 0°–30°S, 0°–20°N, 20°–40°N, 40°–60°N, and 60°–82°N respectively. Panels on the right side indicate the corresponding mean profile differences in percent. The number of coincidences is given in Table 2.

validation studies: within 5 hours in Universal Time, within 5° in latitude and within 10° in longitude. This corresponds to a geographic area of about 500 km by 1000 km at the equator, where the ozone field does not usually exhibit a significant spatial structure, and about 500 km by 500 km poleward of 70° where the ozone field can be very structured at the edge of the polar vortex. The search for the ACE-OSIRIS coincidences has been made for the time period from 9 January 2004 (first usable ACE solar occultation) until 5 August 2004 (last OSIRIS ozone retrieval, version 1.2). The first usable coincidence between the two instruments occurred on 31 January 2004. The latitudinal and temporal distribution of all ACE-OSIRIS coincidences is shown in Figure 1. The majority of the coincidences occurred in the Northern Hemisphere in March–April and July–August, 2004, only 10 coincidences took place between January 31 and mid-February, 2004.

[12] Typical examples of individual coincident ACE and OSIRIS ozone profiles are presented in Figure 2. Relatively smooth profiles are shown in Panel (a) and profiles that have more vertical structure are shown in Panel (b). Clearly, both instruments demonstrate an ability to resolve the vertical ozone structure (Figure 2b). It can be also seen from Figure 2 that the ACE ozone profiles are ~10% smaller at the peak compared to the OSIRIS profiles. Although the individual coincident profiles are shown in the altitude range of 12–48 km, the statistical analysis below is performed only in the range of 16–32 km.

[13] The temporal distribution of the ACE-OSIRIS coincidences is not even but varies significantly with the time of year (Figure 1). Consequently, we performed a statistical analysis of the ACE-OSIRIS coincidences for specific latitude bands rather than on a monthly basis (as in the previous OSIRIS ozone validation studies). ACE and OSIRIS zonal mean coincident ozone profiles in the latitude bands of 0°–30°S, 0°–20°N, 20°–40°N, 40°–60°N, and 60°–82°N, are presented in Figure 3, left-side Panels (a)–(e) respectively. Panels on the right side indicate the corresponding mean profile differences in percent. In addition, the mean ACE-OSIRIS profile differences and their standard deviations are listed in Table 2 for altitudes similar to those in Table 1.

[14] Most of the time, ACE and OSIRIS zonal mean profiles agree within ~4–7% outside the 5–7 km altitude range around the ozone number density peak. In the vicinity of the peak, ACE retrievals are systematically lower than those of OSIRIS by about 10%. Below 18 km, ACE profiles are sometimes larger than OSIRIS profiles by up to 30%. The latter may be due to the possible impact of the high altitude tropospheric clouds or stratospheric aerosols on the ozone measurements by either or both instruments. This assumption is supported by the fact that the difference between the two instruments below 18 km (Figure 3) is larger equatorward of 40°N and smaller poleward of 60°N; this correlates with the decrease in the tropopause height toward the Pole. Another possible reason for the larger differences near 18 km may be due to the fact that the ozone amounts in this altitude range differ by more

Table 2. Same as in Table 1 but for ACE and OSIRIS

Month 2004	# Coinc	Min. Lat., °	Max. Lat., °	Mean Profile Diff., %				STD of Profile Diff			
				21.5 km	23.5 km	25.5 km	27.5 km	21.5 km	23.5 km	25.5 km	27.5 km
Jan/Feb	10	30 S	0	−4.0	−8.2	−7.1	−10.6	7.9	5.4	6.0	3.6
Mar/Jul	35	60 N	83 N	−7.01	−11.8	−7.7	−0.6	7.3	11.6	9.2	12.5
Apr/Aug	16	20 N	40 N	3.5	−0.6	−10.2	−14.8	21.3	15.2	9.9	10.5
Mar/Apr Jul/Aug	42	40 N	60 N	−6.4	−11.0	−14.1	−13.2	15.6	12.6	11.4	10.7
Aug	6	0	20 N	7.2	−4.8	−7.4	−10.8	7.5	14.6	7.8	7.7

than a factor of three and the ozone gradients are steeper. Different OSIRIS and ACE altitude resolution, 1 and 4 km respectively, may also play a role.

[15] As OSIRIS ozone measurements agree well with SAGE III data during the considered time periods (Table 1), a systematic ~10% difference between the ACE and OSIRIS mean coincident profiles around the peak is probably a feature of the ACE-FTS retrievals. A similar systematic difference around the ozone peak has been also detected between the ACE and POAM III, and ACE and SAGE III coincident measurements in March 2004 [*Walker et al.*, 2005], and between the ACE and GOMOS coincident data during mid-February – mid-April and May 2004 [*Fussen et al.*, 2005].

[16] As the ACE field of view is about 4 km, the lower vertical resolution of the ACE measurements could cause the observed systematic underestimation of the ozone concentration around the peak. Any differences in the air mass sampling due to the different ACE and OSIRIS horizontal sampling, 500 and 250 km respectively, and observing geometries, occultation and limb, probably contribute randomly to the differences in the individual coincident profiles and so should average out in the mean profiles. This latter suggestion is supported by the agreement between the OSIRIS limb-measured ozone profiles and ozone data from other solar occultation instruments, SAGE III (Table 1), SAGE II and POAM III [*Petelina et al.*, 2004a, 2004b]. We note that SAGE III vertical resolution is 0.5 km and horizontal sampling is 120 km. The lower vertical resolution of ACE may also be in part responsible to higher ACE-OSIRIS standard deviations compared to OSIRIS-SAGE III standard deviations (Tables 1 and 2).

[17] OSIRIS, SAGE and POAM ozone profiles are retrieved from the measurements in the UV-VIS spectral region while ACE measures ozone at 2–13 microns. Consequently, another possible source of the observed differences in the ozone profiles, particularly near the peak, may be due to uncertainties in the assumed spectroscopic constants used in the ACE ozone retrieval algorithm. This issue is under investigation and will be accounted for in the next version of the ACE Level 2 retrievals. Although there is no evidence for the ACE and OSIRIS misalignment, it is important to note that a 1 km offset in the altitude registration can lead up to 15% difference in the retrieved ozone concentrations.

4. Conclusion

[18] ACE stratospheric ozone profiles, version 1, have been statistically compared with the coincident OSIRIS ozone profiles, version 1.2. All coincidences took place between January 31 and August 5, 2004, with the majority in the Northern Hemisphere. Zonal mean coincident profiles were calculated for several latitude bands between 30°S and 82°N. Statistical comparisons were performed in the altitude range of 16–32 km where OSIRIS ozone data during this time period are in a good agreement, usually better than 6%, with the SAGE III measurement.

[19] At altitudes 3–5 km above and below the ozone peak, ACE-FTS and OSIRIS profiles agree to within ~4–7%. Below 18 km ACE profiles may be up to 30% larger than OSIRIS profiles. These differences are attributed to a possible impact of high altitude tropospheric clouds and stratospheric aerosols, different ACE and OSIRIS vertical resolution, and larger variability and steeper ozone gradients at these altitudes. In the vicinity of the ozone peak the ACE-FTS profiles are systematically about 10% lower than the OSIRIS profiles. This result is consistent for each of the considered 20°–30° latitude bands. As the accuracy of OSIRIS ozone profiles is 5–7%, such systematic difference can be attributed to the lower ACE vertical resolution or to the uncertainties in the ozone spectroscopic constants, particularly in the infrared. Altitude registration is also extremely important for the comparison of individual profiles and can potentially contribute to the differences in these initial comparisons. This paper is intended to show the community the quality of the presently available ACE data and outstanding issues will be addressed in the next version of the ACE Level 2 retrievals.

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