Initial validation comparisons for the Atmospheric Chemistry Experiment (ACE-FTS)

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[1] The Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) is the primary instrument for the ACE satellite mission. The initial validation of ozone profiles from ACE-FTS is based on comparisons with profiles from satellite-borne instruments and balloon-borne ozonesondes. The satellite instruments include the SAGE III and POAM III instruments. The ACE profiles were recorded during March 2004 at high latitudes in the northern hemisphere (>65°N) and were processed with the version 1.0 retrieval algorithm. The ACE-FTS results were found to agree within 10% with those from the other satellite measurements between 15 and 40 km, with ACE-FTS measuring less ozone near the profile maximum. The ACE-FTS has a lower vertical resolution than SAGE III or POAM III and this may contribute to the observed discrepancy. The comparisons with ozonesonde measurements suggest that the ACE-FTS accurately captures vertical structures in the ozone profile that are on the order of several kilometers thick. **Citation:** Walker, K. A., C. E. Randall, C. R. Trepte, C. D. Boone, and P. F. Bernath (2005), Initial validation comparisons for the Atmospheric Chemistry Experiment (ACE-FTS), *Geophys. Res. Lett.*, *32*, L16S04, doi:10.1029/2005GL022388.

1. Introduction

[2] The Atmospheric Chemistry Experiment (ACE) also known as SCISAT-1, a Canadian scientific satellite mission developed for remote sensing of the Earth's atmosphere, was launched on 12 August 2003 [*Bernath et al.*, 2005]. The primary instrument for this mission is a high resolution (0.02 cm^{-1}) Fourier transform spectrometer (ACE-FTS) operating in the infrared region between 750 and 4400 cm^{-1}. This sensor uses the solar occultation technique to determine profiles of atmospheric trace gases, temperature, pressure, and aerosols. The SCISAT-1 satellite is in a circular, 74° inclination low-earth orbit at 650 km, which gives the ACE instruments latitude coverage from approximately 85°N to 85°S with the majority of occultations occurring over the Arctic and Antarctic. One of the primary goals of the ACE mission is to improve our understanding of the chemical and dynamical processes that control the distribution of ozone in the stratosphere and upper troposphere, focusing particularly on the Arctic region [*Wardle et al.*, 1997; *World Meteorological Organization*, 2002]. To do this, accurate measurements of ozone and other species involved in ozone chemistry (such as NO, NO_2, N_2O_5, HNO_3, HCl, $ClONO_2$) are required to determine a detailed ozone budget. Initial validation comparisons for the version 1.0 ACE-FTS profiles have been done with measurements from the Optical Spectrograph and InfraRed Imager System (OSIRIS) [*Petelina et al.*, 2005], Global Ozone Monitoring by Occultation of Stars (GOMOS) [*Fussen et al.*, 2005], HALogen Occultation Experiment (HALOE) [*McHugh et al.*, 2005], Polar Ozone and Aerosol Measurement (POAM) III and Stratospheric Aerosol and Gas Experiment (SAGE) III satellite instruments. This paper describes ozone comparisons that have been made with the POAM III and SAGE III satellite instruments, and also includes qualitative comparisons that have been made with results from balloon-borne ozonesondes. These comparisons focus on the March 2004 period when the ACE-FTS measurements were coincident with both SAGE III and POAM III, and ozonesondes were launched daily from the Eureka, Nunavut (80°N, 86°W) weather station.

2. ACE-FTS Retrievals

[3] Each sunrise or sunset occultation measurement consists of a series of spectra recorded at different tangent heights. The ACE-FTS takes one measurement every 2 seconds, and has a circular field of view of 1.25 mrad, which corresponds to a vertical resolution of 3 to 4 km over most of the altitude range. A two step process is used to retrieve information from the atmospheric spectra (C. D. Boone et al., Retrievals for the Atmospheric Chemistry Experiment Fourier Transform Spectrometer, submitted to *Applied Optics*, 2005). First, spectral lines of carbon dioxide are used to derive the pressure and temperature profiles. Next, these profiles are held fixed and the volume mixing ratio (VMR) profiles for the atmospheric trace gases are determined using a global least squares fitting method. The results are interpolated onto a 1 km grid using a piecewise quadratic method to produce the final product. For version 1.0 of the ACE-FTS retrievals, 80 microwindows in the 1022–2153 cm^{-1} range were used to produce atmospheric profiles of ozone between 10 and 70 km in altitude. The HITRAN 2004 linelist [*Rothman et al.*, 2005] is used in the ACE-FTS retrieval calculations.

3. Comparison Data Sets

3.1. POAM III

[4] POAM III is the third Polar Ozone and Aerosol Measurement instrument to be placed into orbit [*Lucke et*

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al., 1999]. It has nine filtered channels operating in the UV, visible, and near infrared regions. It uses solar occultation to measure vertical profiles of O_3, NO_2, H_2O, and aerosol extinction, with approximately 1 km vertical resolution, and has been in operation since April 1998. Because the SPOT-4 satellite is in a near-polar, sun-synchronous orbit, the POAM III measurements occur in narrow bands at high latitudes with satellite sunrises occurring in the northern hemisphere and satellite sunsets in the southern hemisphere. The ozone retrievals have been validated by comparisons with measurements from HALOE, SAGE II, and ozonesondes and have been found to have an accuracy of ±5% between 13 and 60 km [*Randall et al.*, 2003]. Data from POAM III version 4.0 are used for these comparisons.

3.2. SAGE III

[5] SAGE III measures atmospheric profiles of trace gases and aerosols using solar and lunar occultation [*Thomason and Taha*, 2003]. The measurements are made in 87 spectral channels from 280 to 1545 nm using a grating spectrometer. Vertical profiles of O_3, NO_2, H_2O, NO_3, OClO, temperature, pressure, and aerosol extinction are retrieved from the measurements. The opportunities for solar occultation measurements occur at high latitudes in the northern hemisphere (satellite sunsets) and at mid-latitudes in the southern hemisphere (satellite sunrises), due to the sun-synchronous orbit of the Russian Meteor-3M satellite. Version 3.0 SAGE III data are used for these comparisons. These results have a vertical resolution of ~1 km. Between 15 and 40 km, these retrievals were found to differ by less than 10% when compared to POAM III and HALOE [*Randall et al.*, 2005].

3.3. Ozonesondes

[6] As part of the Canadian Arctic Validation of ACE campaign at Eureka (T. E. Kerzenmacher et al., Measurements of O_3, NO_2 and Temperature During the 2004 Canadian Arctic ACE Validation Campaign, submitted to *Geophysical Research Letters*, 2005), balloon-borne ozonesondes were launched each day at 23h15 UTC from 24 February to 8 March 2004. These measurements provide very high vertical resolution profiles of ozone concentration along the balloon flight path from the ground to an altitude of approximately 30 km. The launch time was typically within 3 hours of the ACE occultation measurement.

4. Satellite Comparisons: POAM III and SAGE III

[7] The following method was used for the satellite comparisons. Pairs of coincident measurements were chosen using 500 km in distance and ±2 hours in time as the criteria. For the latitude range of the measurements (66°–78°N), this distance criterion corresponds to approximately ±4.3° in latitude. Relaxing the time constraint did not significantly increase the number of comparison pairs. Because the measurements occurred during March at high latitudes, maps of potential vorticity were used to exclude those coincidences where the two measurements were sampling different regions of the vortex (i.e. outside versus inside). Thirty pairs of coincident measurements were found for POAM III and ACE-FTS between 16 and 22 March 2004 and, for SAGE III and ACE-FTS, 184 pairs of coincident profiles were found between 1 and 18 March 2004.

[8] For the comparisons, the POAM III and SAGE III profiles were linearly interpolated onto the same 1 km grid as the ACE-FTS profiles. No smoothing was applied to these interpolated profiles. Percent difference profiles were calculated for individual coincidence pairs and then these were averaged to produce average difference profiles. The following equation was used to calculate the individual percent differences:

$$\text{Percent difference} = 100(\text{ACE-FTS} - \textit{comparison}) / [(\text{ACE-FTS} + \textit{comparison})/2], \quad (1)$$

where comparison is the correlative measurement. The number of points included in the averages varied with altitude because of missing data or excluded data. Results from either data set with stated errors of greater than 100% were excluded from the calculations to prevent suspect data from skewing the results. The comparison range was limited to 10–60 km because the data set became much sparser for all instruments below 10 km and the maximum altitude for the POAM III retrievals is 60 km. The ACE-FTS profiles were converted from mixing ratio to number density using the atmospheric density determined from the retrieved temperature and pressure at each altitude. Comparisons with POAM III data were made in both mixing ratio and density units (using Met Office total densities to convert the POAM III data into mixing ratios) and essentially identical average percent difference results were obtained. Therefore only the calculations using number densities are reported in this paper.

[9] The average ozone profiles and average percent difference profiles for ACE-FTS compared to POAM III and SAGE III are shown in Figures 1 and 2, respectively. The error bars given for the average ACE-FTS ozone profiles are the 1-σ standard deviation of the distribution of measurements at each altitude. For the average percent difference profiles, the uncertainty in the mean is shown (i.e. the 1-σ standard deviation of the distribution of differences divided by the square root of the number of coincidences). In general, the initial comparisons of ACE-FTS average profiles with those from POAM III and SAGE III are qualitatively reasonable below 40 km. The ACE retrievals are within 10% of the comparison instruments between 15 and 40 km with ACE-FTS reporting less ozone primarily near the profile maximum. The analysis at this point in time does not indicate significant errors in the altitude registration of the profiles. From 40–55 km, ACE-FTS is higher than POAM III and SAGE III by up to 28% and 38%, respectively; note, however, that these large percent differences correspond to density differences that are only on the order of 5×10^9 cm^{-3} (at 55 km).

[10] One contribution to the discrepancy between the ACE-FTS and other satellite data sets may be the difference in vertical resolution of the retrieved profiles which for the ACE-FTS results is typically 3–4 km whereas for POAM III and SAGE III it is ~1 km. Figure 3 shows two individual comparisons with POAM III showing the difference between the retrieved and interpolated grid for the ACE-FTS measurements. By comparing the two panels, it can be seen

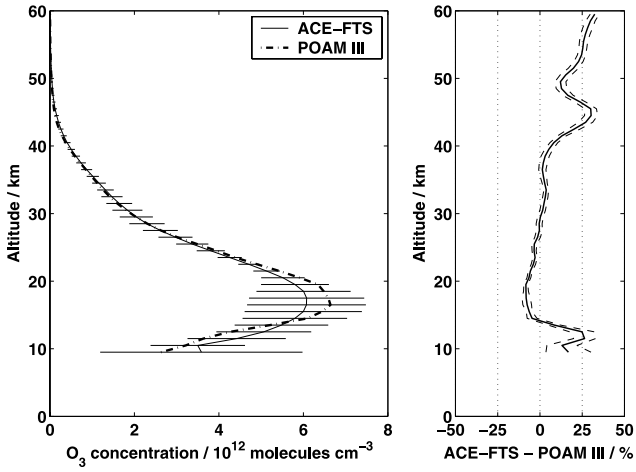

Figure 1. (left) Average profiles of ozone number density from ACE-FTS and POAM III between 16 and 22 March 2004 are shown. 30 profiles are included in each average. The error bars show 1-σ standard deviation of the distribution of ACE-FTS measurements at each altitude. The average latitude of the measurements was 67°N. (right) The average percent difference profile for the ACE-FTS and POAM III comparisons is shown with 1-σ standard deviation of the mean given by the dotted lines.

that the ACE-FTS profile agrees more closely with the POAM III profile when there is a measurement point near the concentration peak maximum (shown in the left hand panel), than when the points nearest the ozone peak are offset from the maximum (as seen in the right hand panel). A simple test was done to examine the effect of the difference in vertical resolution of the measurements. A 5 point moving average was applied to each POAM III profile to crudely reduce the vertical resolution from ∼1 km to ∼4 km and the comparison calculations were repeated. The discrepancies between the POAM III and ACE-FTS profiles were reduced by several percent but were not entirely removed. Further investigations that take into account the actual ACE-FTS field of view and averaging kernels, which vary with altitude, are required. Additionally, the interpolation scheme used in version 1.0 of the ACE-FTS retrievals may have introduced some smoothing of the data thereby lowering the vertical resolution. This has been changed in version 2.0 of the retrievals.

[11] The POAM III and SAGE III instruments measure in the UV/visible region of the spectrum while ACE-FTS makes its measurements in the infrared. Some discrepancies between the retrieved profiles may also arise due to differences in the uncertainties of the spectroscopic parameters between these two regions. For instance, comparisons of ACE-FTS ozone profiles with HALOE (a solar occultation instrument operating in the infrared) show agreement within ±5% between 15 and 35 km [*McHugh et al.*, 2005], rather than as much as −10%, as in the comparisons with POAM III and SAGE III ozone measurements. Note also that in ozone comparisons with two other UV/visible instruments, GOMOS (measuring by stellar occultation) [*Fussen et al.*, 2005] and OSIRIS (recording limb-scattered sunlight) [*Petelina et al.*, 2005], ACE-FTS measures less ozone (5–7% between 15 and 35 km for GOMOS and up to 10% between 15 and 25–30 km for OSIRIS), which are similar to the differences seen in the comparisons with POAM III and SAGE III.

5. Ozonesonde Comparisons

[12] Because of the sparseness of both satellite occultation measurements and balloon-borne ozonesonde measurements, it is difficult to find a sufficient number of coincidences for a statistical study. This situation will improve with continued operation of the ACE mission as more occultation measurements are recorded and made available for comparisons. For this paper, the discussion will be limited to qualitatively comparing the vertical structure in the ozone profiles as observed by ACE-FTS to the much higher resolution profiles measured by balloon-borne ozonesonde instruments.

[13] During the period in March, when ozonesondes were launched daily, there were six ACE-FTS occultation measurements within 200 km of the Eureka weather station. Each occultation was within 3 hours of the coincident launch. An example of one of these comparisons (for March 5) is given Figure 4. In this plot, the ACE-FTS ozone results are shown both on the standard 1 km interpolated grid (grey dashed line) and at the measured tangent points (black dots). From this comparison, it can be seen that the ACE-FTS is sensitive to the "larger" vertical structures in the ozone profile (such as the smaller peak between 10 and 14 km). With a vertical spacing of 3–4 km, ACE-FTS is able to distinguish vertical structures which are at least several kilometers in thickness. It is also interesting to note that in Figure 4, above 10 km, the ozone concen-

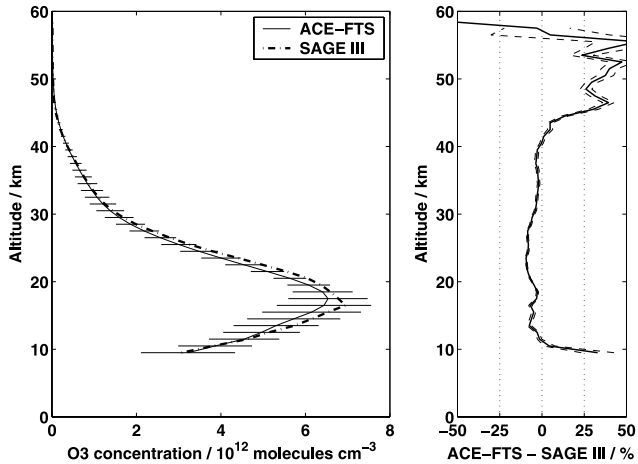

Figure 2. (left) Average profiles of ozone number density for ACE-FTS and SAGE III from 1 to 18 March 2004 are shown. 184 profiles are included in each average. The error bars show 1-σ standard deviation of the distribution of ACE-FTS measurements at each altitude. The average latitude of the measurements was 76°N. (right) The average percent difference profile for the ACE-FTS and SAGE III comparisons is shown with 1-σ standard deviation of the mean given by the dotted lines.

trations at the retrieved tangent points are quite close to the ozonesonde values.

6. Conclusions

[14] The version 1.0 ACE-FTS ozone profiles have been compared to results from the POAM III and SAGE III satellite instruments and balloon-borne ozonesondes. In these initial comparisons, the ACE-FTS agrees within 10% between 15 and 40 km when compared to the two satellite instruments, but systematically reports less ozone near the profile maximum. However, from 40–55 km, ACE-FTS reports more ozone than SAGE III and POAM III by up to 38% and 28%, respectively. Similar discrepancies have been seen in comparisons with other satellite data sets. In comparisons with both OSIRIS [*Petelina et al.*, 2005] and GOMOS [*Fussen et al.*, 2005], ACE-FTS measures less ozone by up to 10% between ~15 and ~30 km. However, when ACE-FTS ozone profiles are compared with HALOE, the discrepancy is ±5% between 15 and 35 km [*McHugh et al.*, 2005]. Above ~40 km, the ACE-FTS reports more ozone than all three of these instruments. A possible source of the discrepancies below 40 km is the difference in vertical resolution of the measurements and this effect is under investigation. There may also be some issues with the spectroscopic parameters used for the retrievals in the different wavelength regions. The ozonesonde comparisons show that the ACE-FTS is able to detect vertical structures, on the order of several kilometers thick, in the ozone profiles. Initial validation comparisons have been made for other species such as HF, HCl, H_2O, CH_4, NO and, NO_2 using the HALOE results [*McHugh et al.*, 2005] and NO_2 using GOMOS results [*Fussen et al.*, 2005]. In general, all of these initial comparisons show that the ACE-FTS retrievals are reasonable between 15 and 40 km. Further work is required to validate the ACE-FTS results at higher altitudes. Improvements, such as increasing the altitude range and including more molecules, will be made in version 2.0 of the ACE-FTS retrieval algorithm.

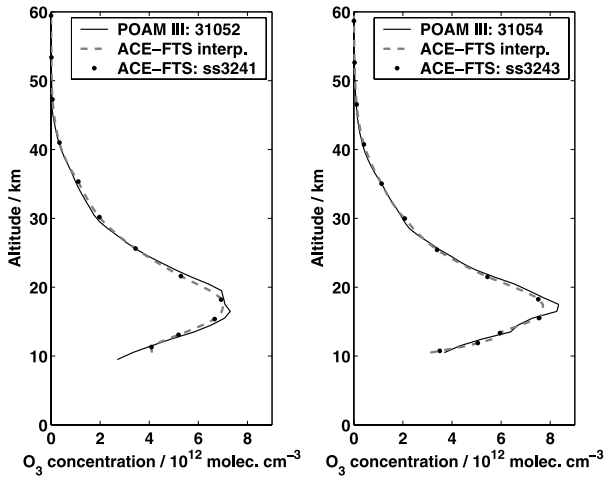

Figure 3. Profile comparisons for two coincidences between ACE-FTS and POAM III are shown to demonstrate the effects of the ACE-FTS altitude sampling. The grey dashed line shows the ACE-FTS retrieval on the 1 km interpolated grid (as reported) and the black points show the retrieved value at each measurement point. (left) Reasonable agreement is achieved at the maximum in ozone concentration when there is a measurement point close to the peak. (right) The agreement is poorer when the measurement points are offset from the peak maximum. The results used for this figure were recorded on 19–20 March 2004 near 67°N.

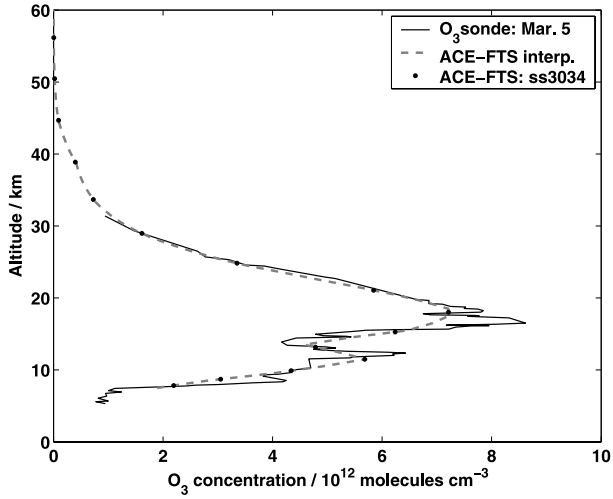

Figure 4. Comparison of ACE-FTS and ozonesonde profiles taken on 5 March 2004 is shown. The grey dashed line shows the ACE-FTS retrieval on the 1 km interpolated grid (as reported) and the black points show the retrieved value at each measurement point. No smoothing has been applied to the ozonesonde profile. The figure shows that the ACE-FTS is sensitive to vertical structure (greater than a few km in thickness) in the measured ozone profile.

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