

Comparison of atmospheric retrievals from ACE and HALOE

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[1] Atmospheric retrievals from ACE are compared to nearly coincident measurements from HALOE. Comparisons are done for O₃, HF, HCl, H₂O, CH₄, NO, NO₂, and temperature. Statistics from 32 profile pairs that were reasonably close in space and time are presented. The temperature retrievals agree to within ± 2 K, an important result as all other retrievals depend on this. ACE gas retrievals are typically higher than HALOE, with the exception of NO and NO₂ where HALOE is higher. This comparison helps provide traceability between two important complementary remote sensing missions, lends confidence to the initial ACE dataset, and provides a baseline for future retrieval improvements. **Citation:** McHugh, M., B. Magill, K. A. Walker, C. D. Boone, P. F. Bernath, and J. M. Russell III (2005), Comparison of atmospheric retrievals from ACE and HALOE, *Geophys. Res. Lett.*, *32*, L15S10, doi:10.1029/2005GL022403.

1. Introduction

[2] The HALogen Occultation Experiment (HALOE) was launched in 1991, and continues to provide vertical profiles of O₃, HF, HCl, H₂O, CH₄, NO, NO₂, temperature, and aerosol extinction at latitudes between $\pm 80^\circ$ [Russell *et al.*, 1993]. In August 2003, the Atmospheric Chemistry Experiment (ACE, also called SCISAT-1) was launched into a similar, but higher inclination orbit [Bernath *et al.*, 2005]. Vertical profiles of 18 gases and temperature are now available in the version 1.0 data release. Both the HALOE and ACE instruments use the solar occultation measurement technique, which provides the important benefit of being virtually self-calibrating. Atmospheric transmission is computed by taking the ratio of the atmospheric and exoatmospheric signals. Gas concentrations are then inverted from the transmission profiles.

[3] Comprehensive HALOE validation results were published for each species in 1996 [Russell *et al.*, 1996a, 1996b; Gordley *et al.*, 1996; Harries *et al.*, 1996; Hervig *et al.*, 1996; Park *et al.*, 1996; Brühl *et al.*, 1996]. Since then, the HALOE algorithm has gone through two major revisions. The HALOE processing version used in this study is the third public release (V19). ACE validation studies concomitant with this work include Walker *et al.* [2005] and Petelina *et al.* [2005] for O₃, and Fussen *et al.* [2005] for O₃ and NO₂. The results presented here will help assess the quality of additional

species in the first available ACE dataset and identify discrepancies that may need further attention.

2. The HALOE Instrument

[4] By viewing the sun through the Earth's limb during spacecraft sunrise and sunset, HALOE records vertical profiles of atmospheric transmission with 4 radiometer channels and 4 dual radiometer/gas-filter correlation channels simultaneously. The instantaneous field of view (IFOV) at the limb tangent point is approximately 2 km vertically by 5 km horizontally. The signals are highly oversampled (< 0.3 km vertical spacing), and after processing the effective vertical resolution is 3–5 km, depending on altitude and channel. From its 57° , 585 km circular orbit, there are nominally 15 sunrises and 15 sunsets every day, equally spaced in longitude. Daily sunrises and sunsets occur in two rather compact latitude bands, sweeping through $\sim \pm 80^\circ$ in just over a month.

[5] The temperature retrieval assumes a CO₂ concentration and matches the 3570 cm⁻¹ transmissions in an upward, hydrostatically-constrained process. This is iterated several times, with intervening profile registrations. Above ~ 85 km temperatures from the MSIS model [Hedin, 1991] are assumed, and below ~ 35 km NCEP temperatures are used. The 1510, 1600 and 1015 cm⁻¹ radiometer channels are used to retrieve NO₂, H₂O, and O₃, respectively, in an onion-peeling fashion. A differential technique is used to retrieve HF, HCl, CH₄, and NO from the 4080, 2940, 2890, and 1900 cm⁻¹ channels. In these channels, the light is split. Half is sent through a cell filled with the target gas, and the other half through a vacuum path. The exoatmospheric difference of these signals is balanced to near the noise level. The difference signal that develops when viewing through the atmosphere is highly sensitive to atmospheric absorption from the target gas, but insensitive to aerosol absorption. The radiometer channels, however, are sensitive to aerosol. To account for this, aerosol extinction is retrieved from the 1900 cm⁻¹ vacuum-path signal and extrapolated to the other channels assuming a sulfate model. The spectroscopy in the HALOE forward model is based on HITRAN 1991–1992, augmented by specific lab measurements in certain regions.

3. The ACE Instrument

[6] ACE tracks the sun during spacecraft sunrise and sunset from a 74° , 650 km near circular orbit, producing a

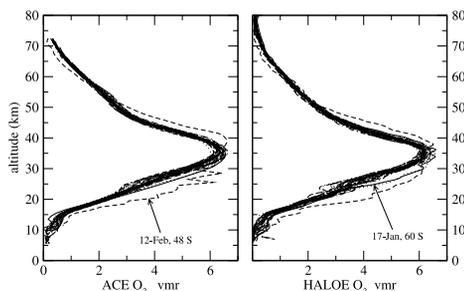


Figure 1. O₃ profiles from the 32 occultation pair coincidences.

coverage pattern similar in most respects to HALOE. The primary instrument on ACE is a Fourier transform spectrometer (FTS), covering 750 to 4400 cm⁻¹ with 0.02 cm⁻¹ resolution. The 1.25 mrad circular IFOV corresponds to ~4 km at the tangent point. The spectrum acquisition time of 2 seconds translates to a tangent point altitude spacing of 3–5 km. ACE also includes a dual visible/near-IR imager, and MAESTRO—a dual spectrograph covering 280 to 1030 nm. In this work, we only examine results from the FTS, and hereafter refer to the ACE-FTS simply as ACE.

[7] Inversion of ACE transmission spectra into vertical profiles of gas volume mixing ratio (vmr) is described by *Boone et al.* [2005]. Briefly, molecular absorption lines are fitted in selected microwindows (typically ~0.3 cm⁻¹ wide) to determine temperature and vmrs. The number and spectral range (in cm⁻¹) of lines used is: 176 CO₂ lines from 933–3739; 54 O₃ lines from 1023–2153; 62 H₂O lines from 1363–3286; 64 CH₄ lines from 1245–2888; 17 NO lines from 1821–1921; 21 NO₂ lines from 1581–1642; 8 HF lines from 3788–4143; 13 HCl lines from 2728–2981. HITRAN 2000 spectral line parameters are used. Processing begins with the temperature retrieval, broken into two altitude regimes. CO₂ lines are simultaneously fit in spectra above 70 km to retrieve CO₂ vmr and temperature. Below 70 km, temperature alone is retrieved using a model CO₂ vmr. A final profile registration is performed, and throughout the process, pressures are constrained by hydrostatic equilibrium. Once the temperature profile is determined, each species' vmr profile is retrieved using simultaneous fits of absorption features from the target gas. The resulting profiles are interpolated onto a 1 km grid.

[8] The earliest retrievals are from Jan. 2004, although many of the early spectra were plagued by ice buildup on the detectors, reducing sensitivity. In addition, because of problems with the version 1.0 retrieval software, only sunset events have been processed.

4. Comparison of Profile Pairs

[9] We searched the ACE and HALOE datasets to find pairs of events for which a meaningful comparison could be made. We discounted any profiles separated by more than 500 km or 4 hours and eliminated seven profiles because of the aforementioned ice buildup. The remaining 32 profile pairs were as follows: 29 from 4–10 July 2004 near 64°N; 2 from 17 Jan. 2004 near 60°S; 1 from 12 Feb. 2004 near 47°S. All occultations in this collection were spacecraft sunsets. Time differences were less than 127 minutes, with an average of 55 minutes. The largest separation was

498 km, and the average was 284 km. The maximum latitude difference was 2°, but neither ACE nor HALOE was predominantly higher or lower in latitude.

[10] Figure 1 shows the O₃ profiles used in this study. The two profile pairs from Jan. and the single pair from Feb. stand out slightly from the 29 July pairs. Comparisons of all species were carried out both with and without these three pairs, but no significant difference was found, except for where polar mesospheric cloud (PMC) interference skewed the HALOE retrievals, as we discuss below. The results that follow include all 32 profile pairs. To compare the datasets, the HALOE profiles were interpolated onto the 1 km ACE altitude grid. Only altitudes where both HALOE and ACE had valid retrieval results for all 32 profiles were retained.

[11] Figure 2 shows comparisons of all seven gas species and temperature. Mean HALOE and ACE profiles are shown in the left panels. The right panels contain the mean difference and root mean square (rms) difference profiles. The mean profiles have uncertainty values indicated with horizontal bars. For ACE, these are 1-sigma statistical errors calculated during the retrieval process and do not include any estimate of systematic errors. Estimates of combined random and systematic errors were provided by the HALOE project team (E. Remsburg, personal communication, 2004). The uncertainties depicted are for individual profiles. The

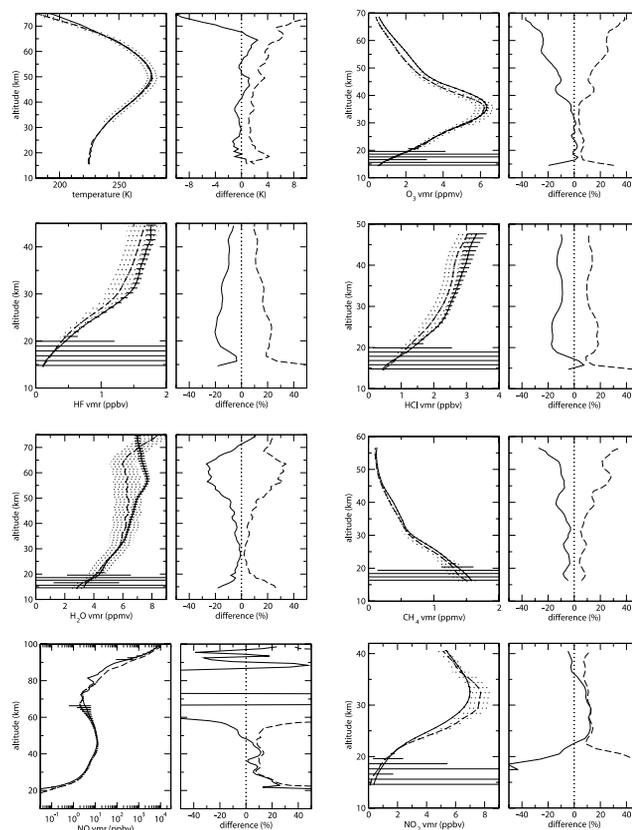


Figure 2. Comparison results. *Left panels:* mean ACE (solid) and HALOE (dashed) retrievals. Horizontal error bars indicate the average single-profile uncertainty. *Right panels:* mean difference (solid) and rms difference (dashed). For the gas species, relative differences are 100% × (HALOE–ACE)/HALOE. For temperature, the absolute HALOE–ACE difference is computed.

random component of the error will be diminished by averaging, so these may be up to $\sqrt{32}$ times too large, since the profiles in Figure 2 are averages. ACE error bars for NO are omitted in the 68–90 km region for clarity. In this region, the fractional uncertainty of the NO retrieval (for both HALOE and ACE) grows because of the large thermospheric overburden and possible variations from auroral or solar activity.

[12] Although the profile pairs are separated by relatively large distances, the high latitude summer conditions sampled here are generally benign and stable, with the important exception of the upper mesosphere, where PMCs can occur. HALOE temperature and H₂O are affected by these clouds, and for this reason we limit the comparison to 75 km and below [McHugh, 2003]. Still, the differences seen in Figure 2 from 70–75 km appear to be from residual PMC contamination in the HALOE retrievals. In the Feb. profile pair—the only pair where PMCs could not occur—no bias at 75 km is evident.

[13] In addition to PMCs causing localized atmospheric variability, many species normally exhibit latitudinal gradients. However, since neither instrument was consistently higher or lower in latitude for the occultation pairs used here, this should not affect the mean differences. Natural variability is also found near the day-night terminator, where photochemically active molecules such as NO₂, NO, and O₃ exhibit twilight gradients. This is modeled in the HALOE retrieval, but ACE does not yet include any such correction. While the diurnal correction can be significant (particularly for lower stratospheric NO₂ measured at local sunrise) for the cases considered here it is negligible. Nearly all the occultations in this study occurred at high beta angle and in the polar summer, where diurnal effects are less pronounced. This was confirmed by comparisons of HALOE retrievals with and without the diurnal correction.

[14] In the initial HALOE validation studies (references given in section 1) HALOE was compared to a number of instruments, including ATMOS, an infrared FTS solar occultation experiment similar to ACE. There are striking similarities in the comparisons. ACE-HALOE differences for O₃, HCl, HF, H₂O, and CH₄ (Figure 2) are nearly identical to the ATMOS-HALOE differences. Results were somewhat different for NO and NO₂, but only a single ATMOS occultation was used for these species. ATMOS temperatures were not compared to HALOE. Other instruments were compared to HALOE and showed different behavior, but the ATMOS-HALOE results are mentioned here because of the similarity between the ATMOS and ACE instruments.

5. Summary

[15] Using 32 nearly coincident ACE and HALOE occultation measurements, version 1.0 ACE retrievals were compared to version 19 HALOE retrievals. Temperatures agree to within ~ 2 K, with ACE slightly colder than HALOE below 40 km, and slightly warmer above. While this is indicative of a slight registration discrepancy, it is well within the combined uncertainty of the instruments. ACE vmrs are up to 20% higher than HALOE, except for NO and NO₂, where HALOE is higher. Table 1 summarizes the differences.

Table 1. Comparison Results

Species	ACE-FTS Behavior as Compared to HALOE
T	± 2 K from 35 to 70 km ~ 10 K warmer at 75 km (PMC contamination)
O ₃	$\pm 5\%$ from 15 to 35 ~ 0.4 ppmv higher from 35 to 70 km
HF	10–20% higher throughout (15 to 45 km)
HCl	$\pm 10\%$ below 20 km 10–20% higher from 20 to 48 km
H ₂ O	0–20% higher below 20 km 0–10% higher from 20 to 45 km 10–30% higher above 45 km
CH ₄	$\sim 10\%$ higher throughout (18 to 55 km)
NO	10–20% lower from 25 to 55 km (large uncertainties from 65 to 90 km) $\sim 50\%$ lower above 90 km
NO ₂	0–50% higher below 22 km 0–10% lower from 22 to 35 km

[16] These comparisons are preliminary in several important respects. The coincident pairs are predominantly from a single season and latitude, and all are orbital sunsets. Also, the spatial separations of the occultation pairs are sometimes large, ranging up to 500 km. A more complete intercomparison using closer measurement pairs from more diverse conditions—including both sunrises and sunsets and a variety of seasons and latitudes—is desirable, but not yet possible. An updated ACE processing version is under development, but because version 1.0 is publicly available and will be used in a variety of science studies, it is important to characterize it to the extent possible. Similarly, a newer version of the HALOE retrieval is being developed, and the updated datasets should be compared when available.

[17] Because HALOE has an extensive data record and has been characterized against many other instruments, this intercomparison helps put ACE in context with the larger community of atmospheric remote sensing measurements. In particular, the temperature retrieval agreement is an important indicator of the health of the overall ACE dataset. In general, these comparisons lend confidence to the first release of ACE products, and may help guide future retrieval efforts for both instruments.

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References

- Bernath, P. F., et al. (2005), Atmospheric Chemistry Experiment (ACE): Mission overview, *Geophys. Res. Lett.*, 32, L15S01, doi:10.1029/2005GL022386.
- Boone, C., R. Nassar, K. Walker, Y. Rochon, S. McLeod, C. Rinsland, and P. Bernath (2005), Retrievals for the Atmospheric Chemistry Experiment Fourier Transform Spectrometer, *Appl. Opt.*, in press.
- Brühl, C., et al. (1996), Halogen Occultation Experiment ozone channel validation, *J. Geophys. Res.*, 101(D6), 10,217.
- Fussen, D., F. Vanhellefont, J. Dodiin, C. Bingen, K. Walker, C. Boone, S. McLeod, and P. Bernath (2005), Intercomparison of ozone and nitrogen dioxide number density profiles retrieved by the ACE and GOMOS occultation instruments, *Geophys. Res. Lett.*, doi:10.1029/2005GL022468, in press.

- Harries, J. E., J. M. Russell III, A. F. Tuck, L. L. Gordley, P. Purcell, K. Stone, R. M. Bevilacqua, M. Gunson, G. Nedoluha, and W. A. Taub (1996), Validation of water vapor measurements from the Halogen Occultation Experiment, *J. Geophys. Res.*, *101*(D6), 10,205.
- Hedin, A. E. (1991), Extension of the MSIS thermosphere model into the middle and lower atmosphere, *J. Geophys. Res.*, *96*(A2), 1159.
- Hervig, M. E., et al. (1996), Validation of temperature measurements from the Halogen Occultation Experiment, *J. Geophys. Res.*, *101*(D6), 10,277.
- Gordley, L. L. (1996), et al., Validation of nitric oxide and nitrogen dioxide measurements made by the Halogen Occultation Experiment for UARS platform, *J. Geophys. Res.*, *101*(D6), 10,241.
- McHugh, M. J., M. Hervig, B. Magill, R. Thompson, E. Remsberg, J. Wrotny, and J. Russell III (2003), Improved mesospheric temperature, water vapor and polar mesospheric cloud extinctions from HALOE, *Geophys. Res. Lett.*, *30*(8), 1440, doi:10.1029/2002GL016859.
- Park, J. H., et al. (1996), Validation of Halogen Occultation Experiment CH₄ measurements from the UARS, *J. Geophys. Res.*, *101*(D6), 10,183.
- Petelina, S. V., E. J. Llewellyn, K. A. Walker, C. D. Boone, P. F. Bernath, R. L. Gattinger, D. A. Degenstein, and N. D. Lloyd (2005), Validation of ACE-FTS stratospheric ozone profiles against Odin/OSIRIS measurements, *Geophys. Res. Lett.*, *32*, L15S06, doi:10.1029/2005GL022377.
- Russell, J. M., III, L. Gordley, J. Park, S. Drayson, W. Hesketh, R. Cicerone, A. Tuck, J. Frederick, J. Harries, and P. Crutzen (1993), The Halogen Occultation Experiment, *J. Geophys. Res.*, *98*(D6), 10,777.
- Russell, J. M., III, et al. (1996a), Validation of hydrogen fluoride measurements made by the Halogen Occultation Experiment from the UARS platform, *J. Geophys. Res.*, *101*(D6), 10,163.
- Russell, J. M., III, et al. (1996b), Validation of hydrogen chloride measurements made by the Halogen Occultation Experiment from the UARS platform, *J. Geophys. Res.*, *101*(D6), 10,151.
- 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.*, doi:10.1029/2005GL022388, in press.

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