Comparison of Column Abundances from Three Infrared Spectrometers During AASE II

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Abstract

Three Fourier transform infrared (FTIR) spectrometers were on board the NASA DC-8 during the second Airborne Arctic Stratospheric Expedition (AASE II) in 1992. Two FTIRs used solar absorption and one used thermal emission. We compare over 2000 measurements from these 3 FTIRs, on 12 DC-8 flights, for closely coincident air masses and times, both inside and outside the polar vortex. In the majority of cases the offset biases are quite small, in the range 1-4%, and comparable to the absolute precisions expected. In most cases the rms scatter is in the range 4-11%; this scatter is unlikely to be geophysical, but rather is probably instrumental or analytical in origin.

Introduction

In this paper we compare results from the 3 FTIR spectrometers on board the NASA DC-8 during the AASE II campaign in 1992. The overall scientific goals of the AASE II campaign [*Anderson and Toon*, 1993] were to investigate both the potential for ozone loss in the Arctic during the coming decade, and contemporary ozone loss at northern mid-latitudes. A suite of 13 instruments was therefore assembled to make measurements.

Instruments

SAO FTIR

This spectrometer, also called the far-infrared spectrometer (FIRS-2), was built at the Smithsonian Astrophysical Observatory (SAO), and has flown on 9 balloon flights from 1987 through 1994, plus 19 DC-8 flights for AASE II. The instrument, data analysis, and calibration are discussed in *Traub et al.* [1991, 1994], *Abbas and Traub* [1992], and *Johnson et al.* [1995]. The SAO FTIR simultaneously measures in the far-infrared (80–200 cm^{-1}) with apodized resolution 0.008 cm^{-1}, and, on these flights, 0.024 cm^{-1} in the mid–infrared (350–700 cm^{-1}). The instrument measures a thermal emission spectrum. The atmosphere is viewed at 7 elevation angles from 0°to 32°(corrected for aircraft roll angle), plus 2 calibration scans, in an 11-min cycle. The viewing azimuth is +90°from the aircraft heading, i.e., through a right (starboard) side window opening.

For each species, from 1 to 17 microwindows are selected, and a least-squares spectral-line fitting analysis is done. Initial volume mixing ratio (*vmr*) profiles are taken from standard mid-latitude ATMOS results, with the secularly-increasing species (HF and HCl) updated to 1992. Temperature and pressure profiles are from National Meteorological Center (NMC) data, for the time and location of the DC-8.

In each observing sequence, HF is analyzed first, by allowing the initial HF profile (vmr_0) to be scaled vertically, to model the effect of subsidence, using the simple law $vmr(z) = vmr_0[(1+s)z]$, where s is the (dimensionless) subsidence factor [*Toon et al.*, 1992]. Estimated subsidences from each of the upper 4 elevation angles are combined to form a weighted mean. This is then used for the analysis of all other species in the same observing sequence. For these other species, the subsided model profiles are scaled in amplitude. The purpose of this two-step model process is to separate the effects of dynamics and chemistry.

JPL FTIR

The JPL spectrometer, also called the MkIV interferometer, was designed and built at the Jet Propulsion Laboratory (JPL). It has operated on the ground at McMurdo Station in 1986; on the DC-8 in 1987, 1989, and 1992; and has performed 7 successful balloon flights from 1989 through 1994. The instrument and data reduction technique are described in *Toon et al.* [1989, 1991, 1992]. The entire 650 to 5450 cm^{-1} spectral range is measured simultaneously at an apodized resolution of 0.02 cm^{-1} on the DC-8. One spectrum is recorded every 50 sec. The instrument measures the solar spectrum from the center of the disc, with atmospheric absorption superposed. The DC-8 is typically flown on a path which keeps the solar elevation angle in an optimum range (2 to 5°) as long as possible (1 to 2 hr.). A sun tracker is used for elevation and azimuth pointing correction. The viewing azimuth is -85 to $-95°$ from the aircraft heading, i.e., out the left (port) side.

Spectra are averaged in groups of 5 to 15; up to 15 microwindows per species are analyzed using least-squares spectral-line fitting. Initial model *vmr* profiles are from standard mid-latitude ATMOS results, with HF and HCl updated to 1992. Analyses are performed using 2 atmospheric temperature/pressure profiles, one for warm mid-latitudes and one for a cold high latitudes. The actual atmosphere used is a linear interpolation between these two using the NMC temperature at the time and location of the measurement.

For the AASE II flights, HF is analyzed first, not by scaling the amplitude of the *vmr* profile, but by allowing the profile to be compressed vertically, using the subsidence relation given above. For other species, the subsided profiles are scaled in amplitude. In these respects, the JPL and SAO procedures are the same.

NCAR FTIR

This spectrometer was built by the National Center for Atmospheric Research (NCAR) around an Eocom modulator and has flown on over 200 flights of the NCAR Saberliner, NASA P3, Electra and DC-8 aircraft from 1978 through 1993. The instrument and data acquisition are discussed in *Mankin* [1978], *Mankin and Coffey* [1989], *Coffey et al.* [1989], and *Mankin et al.* [1990]. The spectral range is 700 to 5000 cm^{-1}; the apodized resolution is 0.06 cm^{-1}. Each spectrum requires 6 sec to record. The instrument measures solar emission and atmospheric absorption, and uses a sun tracker in an elevation range -2 to 15°. The viewing azimuth is -75 to $-105°$ from the aircraft heading, i.e., the left (port) side.

Spectra are averaged in groups of 10, and 1 to 4 spectral regions per species are used. Data analysis methods are noted in *Gaines et al.* [1993]. Briefly, for HF and HCl an equivalent width method is used, such that the depth of the target absorption feature is measured, and the corresponding line of sight column abundance is determined using a precomputed curve of growth. For O_3 and HNO_3 a least-squares spectral line fitting program (SFIT) is used [*Rinsland et al.*, 1982]; for H_2O an interactive method is used to adjust a calculated spectrum to match the observed spectrum.

The model *vmr* profiles for HF, HCl and HNO_3 are mid-latitude ones from *Coffey et al.* [1989]; O_3 is from *Mankin and Coffey* [1989]; H_2O is from *Smith* [1982], lowered by 4 km in the Arctic; temperature and pressure are from *Barnett and Corney* [1985]. The columns reported in the

AASE-II CD-ROM are vertical integrals above the aircraft altitude, except for H_2O which is reported as the integrated column above 200 mb; for H_2O the values reported here differ from the CD-ROM in that they are columns above the aircraft.

For all species, the adjustable parameter is the *vmr* amplitude scaling factor. In particular, except for the 4 km offset for H_2O mentioned just above, the profiles are not adjusted vertically.

Comparison Method

To compare results from the SAO, JPL, and NCAR FTIRs, we compiled all overlap species during all common measurement periods. The data are displayed in Figure 1. The overlap species are HF, HCl, O_3, HNO_3, and H_2O. With the single exception of NCAR H_2O, all the data presented here have already been published in the AASE II CD-ROM [*Gaines et al.*, 1993]. The 1992 UT date at the beginning of each flight, and the length of each common observing period (in 10^3 sec) is as follows: January 14(8), 16(3), 19(12.5), 22(16); February 17(9), 20(5.5), 22(14); March 10(7.5), 12(6.5), 14(8.5), 18(11), and 20(8). The number of observations used are SAO, 690; JPL, 615; and NCAR 732. The totals are 2037 observations over 30.4 hours.

All of the observations in Figure 1 were carried out between the latitudes of 50 and 84°N, and longitudes from 20°E to 140°W, except for the February 20 run at about 20°N and 67°W near Puerto Rico. Observations were made both inside the Arctic vortex (characterized by large HF columns) and outside the vortex (small HF columns). This wide range of conditions gives rise to a correspondingly large dynamic range in column abundances, with a factor of about 4 for HF and HCl, a factor of 3 for O_3, and a factor of about 2 for HNO_3 and H_2O. The 3 FTIRs track these dynamic swings quite well, with few exceptions.

In each panel in Figure 1, we determine a time series of median values by computing the median of all data points in a sliding window of width 3000 sec. If there are fewer than 5 points in any window, the width is increased until this threshhold is reached. The resulting time series is then fit with a cubic polynomial (lower order in the shortest 2 panels). The resulting curve follows closely the one that might be drawn by eye.

Comparison Statistics

We define the relative deviation of a measurement as

$$\text{relative deviation} = (\text{data} - \text{median})/\text{median},$$

where "median" refers to the smooth median trend line at the time of the data point. For each instrument and species combination we calculate the relative deviation of each data point; we define the offset bias to be the average of these values, for all 12 flights together. The offset bias values are collected in Table 1; a positive offset means that the value exceeds the median.

Table 1. Offset bias: FTIRs on DC-8 (12 flights)

Species	SAO (%)	JPL (%)	NCAR (%)
HF	12	−2	−13
HCl	1	1	1
O_3	3	2	− 3
HNO_3	9	−6	− 2
H_2O	4	4	−12

Table 2. RMS deviation: FTIRs on DC-8 (12 flights)

Species	SAO (%)	JPL (%)	NCAR (%)
HF	10	4	16
HCl	11	7	11
O_3	8	4	5
HNO_3	21	5	9
H_2O	9	7	11

We also calculate a root-mean-square (rms) deviation for each instrument and species combination. This rms is defined as the square root of the average of the squares of the difference between each data point and the median-plus-single-flight offset bias. The rms values are collected in Table 2.

Discussion

From Table 1 we see that the offsets fall in 2 groups. In the first group, with 67% (10/15) of the entries, the offsets are small, in the range 1–4%. This is typical of what might be expected from systematic errors in spectroscopic parameters, zero levels, or gains.

The species HCl and O_3 show offset biases of 1–3%. Since it is unlikely that biases this small would occur by chance, we suggest that this represents an estimate of the true inter-instrumental differences. (Note that the biases (e.g., HCl) do not have to sum to zero, as they are measured with respect to a median, not an average.)

The remaining biases are larger, in the range 6–13%. We briefly consider each of these.

The SAO HF columns are about 12% larger the median, which could be caused by either a line-broadening parameter which is too small (since the HF line is saturated), or the fact that the SAO instrument always viewed a more polar airmass than the others. To test the latter hypothesis, we used potential vorticity (PV) maps to determine the difference in effective PV seen across a span of 170 km (50 km to starboard plus 120 km to port), and a measure of the empirical gradient at a typical vortex wall point [*Traub et al.*, 1994]; we found that the SAO HF should tend to be about 2% larger than the other instruments, which is insufficient to explain the observed difference.

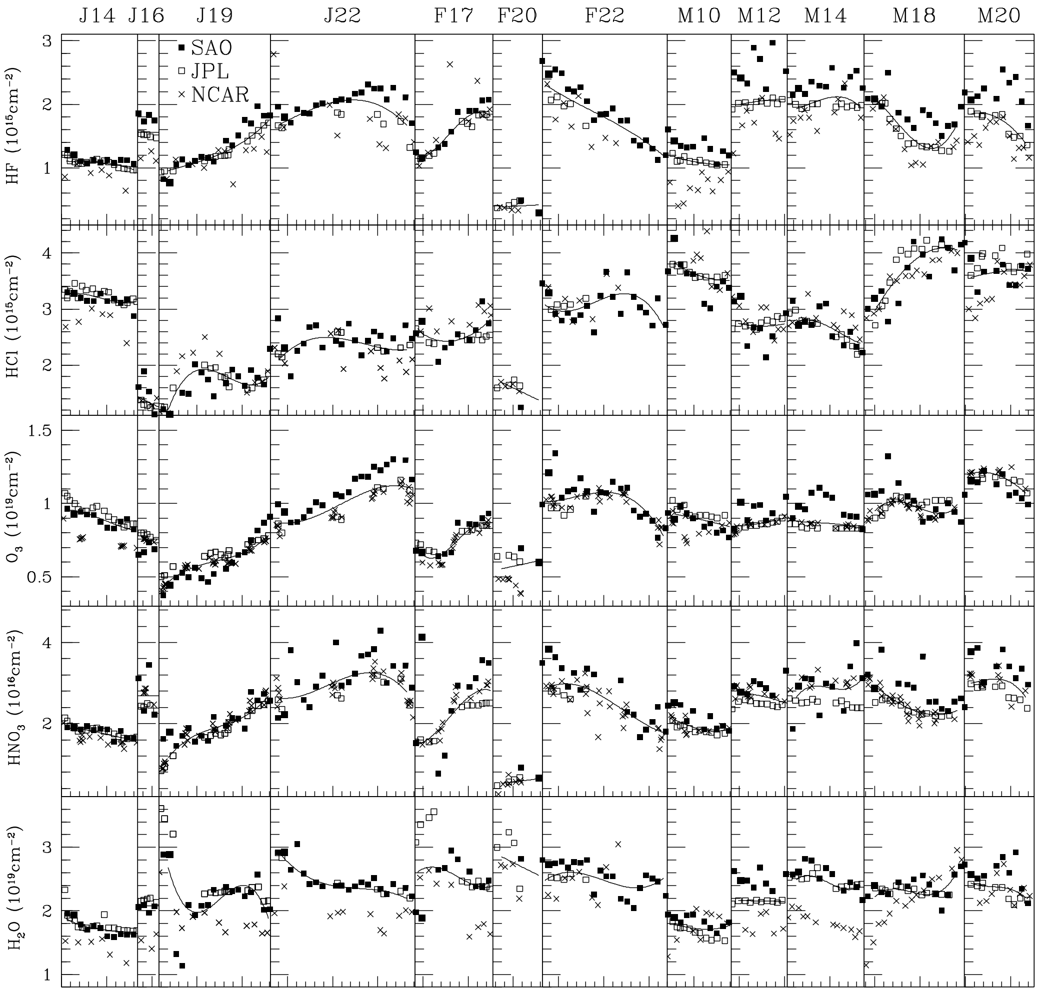

Figure 1. Column abundances of HF, HCl, O_3, HNO_3, and H_2O, during the AASE II campaign in January, February, and March 1992, as measured on the DC-8 by 3 FTIRs: SAO (solid square), JPL (open square), and NCAR (4-point star). Abscissa tics are 1000 sec. The smooth line in each panel is the median trend.

The SAO HNO_3 column is about 9% above the median, which could be due to causes similar to those for HF, but in this case there is an additional factor of relatively high scatter due to reduced signal-to-noise in this channel, which may make the absolute calibration correspondingly uncertain.

There is an 11% difference on average between the NCAR and JPL columns of HF, with NCAR giving the smaller values. Both of these instruments have essentially the same line of sight and air mass, and use the same spectral line. Differences in analysis are the most likely cause of the offset. In particular, differences in treatment of the profile may contribute much of the discrepancy: JPL squashes its profile vertically, whereas NCAR multiplies its profile by a constant at all altitudes. In a previous (unpublished) comparison of JPL and NCAR spectra from a 1989 AASE I DC-8 flight, it was found that the bias was substantially reduced when a single analysis package was used, clearly indicating that analytical methods can be an important source of bias.

The NCAR H_2O column is about 16% smaller than the SAO and JPL values. Since the aircraft often flew close to the hydropause, we sometimes had tropospheric water in our line of sight. The water *vmr* has a very steep vertical gradient below the hydropause. It is possible that differences in modeling this component are the cause of part of the bias.

Inspection of Figure 1 and Table 1 together shows that the biases are not the same from day to day. We have no explanation for this drift.

The rms scatter entries in Table 2 show that in 13 of 15 cases (87%) the rms is in the range 4–11%. The 2 other cases are the relatively large values for the SAO HNO_3, which was noted above as being in a low signal-to-noise band during these flights, and the NCAR HF, which tends to have significant outlier points.

For AASE I, *Toon et al.* [1992] showed that derived abundance variations due to geophysical fluctuations were small compared to the measurement precision; thus 50-sec observations were averaged in larger groups with little loss of information. (Inspection of Figure 2 in *Toon et al.* [1992] shows that the rms scatter in AASE I was comparable to that in AASE II, so the 2 JPL data sets can be compared.) This suggests that the rms deviations in Table 2 are not atmospheric in origin.

Conclusion

We compared the results of 3 FTIR instruments on the DC-8, measuring 5 species in common over a period of about 30 hours, distributed over 12 flights during the AASE II campaign. The meteorlogical conditions varied significantly, from inside the polar vortex to well outside. The columns of each species varied dramatically, by factors of 2 to 4. We removed the dominant trend in column abundance for each day by subtracting a smooth median from the individual observations. In the majority of cases the systematic offsets are quite small, 1–4%. The rms scatter exceeds the atmospheric variation, and is probably due to instrumental or analytical effects. Overall, the comparison shows that there is a large degree of agreement between the instruments, but that improvements might yet be made in some areas.

The present paper is limited to comparing results which were obtained and analyzed independently by 3 groups. In future comparisons, it might be worthwhile having more communication between groups at an earlier stage to minimize systematic differences in modeling. With this caveat, it is hard to imagine a better set of conditions for comparison than existed on these flights.

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References

Abbas, M. and W. A. Traub, Stratospheric minor constituent distributions from far-infrared thermal emission spectra, *J. Geophys. Res., 97,* 18035-18045, 1992.

Anderson, J. G., and O. B. Toon, Airborne arctic stratospheric expedition II: an overview, *Geophys. Res. Lett., 20,* 2499-2502, 1993.

Barnett, J. J. and M. Corney, Middle atmosphere reference model derived from satellite data, *Handbook for MAP, 16,* 47-85, University of Illinois, 1985.

Coffey, M. T., W. G. Mankin, and A. Goldman, Airborne measurements of stratospheric constituents over Antarctica in the austral spring 1987, 2. halogen and nitrogen trace gases, *J. Geophys. Res., 94,* 16597-16613, 1989.

Gaines, S., P. Hathaway, and S. Hipskind, eds., AASE II CD-ROM, NASA/UARP-004, Edition 2, NASA Ames Research Center, 1993.

Johnson, D. G., K. W. Jucks, W. A. Traub, and K. V. Chance, Smithsonian stratospheric far-infrared spectrometer and data reduction system, *J. Geophys. Res.,100,* 3091–3106, 1995.

Mankin, W. G., Airborne Fourier transform spectroscopy of the upper atmosphere, *Opt. Eng., 17,* 39-43, 1978.

Mankin, W. G. and M. T. Coffey, Airborne measurements of stratospheric constituents over Antarctica in the austral spring 1987, 1. Method and ozone observations, *J. Geophys. Res., 94,* 11413-11421, 1989.

Mankin, W. G., M. T. Coffey, A. Goldman, M. R. Schoeberl, L. R. Lait, and P. A. Newman, Airborne measurements of stratospheric constituents over the Arctic in the winter of 1989, *Geophys. Res. Lett., 17,* 473-476, 1990.

Rinsland, C. P., A. Goldman, F. J. Murcray, D. G. Murcray, M. A. H. Smith, R. K. Seals, Jr., J. C. Larsen, and P. L. Rinsland, Stratospheric N_2O mixing ratio profile from high-resolution balloon-borne solar absorption spectra and laboratory spectra near 1880 cm-1, *Appl. Opt., 21,* 4351-4355, 1982.

Smith, M. A. H., Compilation of atmospheric gas concentration profiles from 0 to 50 km, NASA TM 83289, 1982.

Toon, G. C., C. B. Farmer, L. L. Lowes, P. W. Schaper, J.-F. Blavier and R. H. Norton, Infrared aircraft measurements of stratospheric composition over Antarctica during September 1987, *J. Geophys. Res., 94,* 16571-16596, 1989.

Toon, G. C., The JPL MkIV interferometer, *Optics and Photonics News, 2,* 19-21, 1991.

Toon, G. C., C. B. Farmer, P. W. Schaper, L. L. Lowes, and R. H. Norton, Composition measurements of the 1989 arctic winter stratosphere by airborne infrared solar absorption spectroscopy, *J. Geophys. Res., 97,* 7939-7961, 1992.

Traub, W. A., K. V. Chance, D. G. Johnson, and K. W. Jucks, Stratospheric spectroscopy with the far-infrared spectrometer (FIRS-2): overview and recent results, *SPIE, 1491,* 298-307, 1991.

Traub, W. A., K. W. Jucks, D. G. Johnson, and K. V. Chance, Subsidence of the Arctic stratosphere determined from thermal emission of HF, *J. Geophys. Res., 100,* 11,261–11,268, 1995.

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