

Evaluation of the ACE FTS for obtaining nadir measurements

Eldon Puckrin^{*a}, Wayne Evans^b, Chris Ferguson^b, Kaley Walker^c and Denis Dufour^d

^aDefence R&D Canada (DRDC) – Valcartier, 2459 Pie-XI Blvd N., Val-Bélair, QC, G3J 1X5

^bTrent University, Environmental Resource Studies, Peterborough, ON, K9J 7B8

^cUniversity of Waterloo, Dept. of Physics, 200 University Ave. W., Waterloo, ON, N2L 3G1

^dUniversity of Toronto, Dept. of Physics, 255 Huron St., Toronto, ON, M5S 1A1

ABSTRACT

The SciSat-1 mission is a dedicated Canadian science satellite that will investigate processes that control the distribution of ozone in the stratosphere. The SciSat-1 satellite consists of primarily two science instruments; an Atmospheric Chemistry Experiment (ACE) high-resolution Fourier-transform spectrometer (FTS), and an ultraviolet/visible/near-infrared spectrograph. These instruments will primarily function in occultation mode; however, during the dark portion of the orbit the Earth will pass between the Sun and the satellite. This configuration will give rise to the opportunity of acquiring some nadir-view FTIR spectra of the Earth. Since the ACE FTS was designed to view a hot source (i.e., the Sun) at high resolution using a single scan, it is necessary to determine if the FTS will provide nadir spectra of the relatively cold atmosphere and surface with a sufficient signal-to-noise ratio. Methane, ozone and carbon monoxide gases were used in the cell for the purpose of determining the measurement characteristics of the ACE FTS instrument for a low-intensity source. These measurements were compared with data obtained from the Interferometric Monitor for Greenhouse (IMG) gases onboard the ADEOS satellite. The results show that the ACE FTS should be able to measure the abundant trace gases in the atmosphere with sufficient signal-to-noise ratio.

Keywords: satellite remote sensing, occultation, FTIR, ozone, nadir, column amount, air pollution, greenhouse gases

1. INTRODUCTION

The SciSat-1 satellite was launched successfully on August 12, 2003 carrying the Atmospheric Chemistry Experiment (ACE). The satellite consists primarily of two science instruments, the ACE Fourier-transform spectrometer (FTS), shown in Figure 1A, and an optical spectrograph for the Measurement of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation (MAESTRO). SCISAT-1 uses the occultation of the Sun by the Earth to make detailed determinations of the structure and chemistry of the atmosphere in heights ranging from 4 to 100 kilometres above the Earth's surface. The satellite orbits the Earth 15 times each day providing an opportunity to observe sunlight which has passed through the Earth's atmosphere during 15 brief "sunrises" and "sunsets", resulting in 30 sets of observations each day.

However, in between the sunset and sunrise occultation, the ACE FTS will be pointed at the dark-side of the Earth, as shown in Figure 1B, and therefore, will be capable of acquiring and storing nadir spectra of the Earth's atmosphere. This will result in another set of atmospheric gas measurements, i.e., column gas amounts, which can be made for each satellite orbit¹. These column gas measurements will provide similar information to those measured by the Interferometric Monitor for Greenhouse (IMG) gases, which operated for about six months in 1997 onboard the ADEOS satellite². Thus, the nadir-view data could potentially contribute extra science to the ACE mission. For example, radiative trapping or the absorption of upwelling thermal radiation by the atmosphere can be observed for several greenhouse gases. This type of information is important to verify that climate models are correct in the forcing function aspect³⁻⁵. In addition, column amounts are useful for determining the presence of localized sources of pollution⁶. The nadir data measured with the ACE instrument would be very useful to fill in spatial gaps between occultations in the measurement of several stratospheric gases, particularly ozone. The potential science for future nadir missions could be evaluated as well. In the past we have measured the radiative trapping from CFC11 and CFC12 from IMG spectra. The

* eldon.puckrin@drdc-rddc.gc.ca; phone 418 844-4000; fax 418 844-4511

radiative trapping from ozone, methane, nitrous oxide and carbon dioxide also can be easily measured with good signal-to-noise from the IMG spectra, and column amounts of these gases can be measured from the same data.

Since the ACE FTS was designed to view a hot source (i.e., the Sun) at high spectral resolution using a single scan, it is necessary to determine if the FTS will provide nadir spectra of the relatively cold atmosphere and surface (~ 300 K) with a sufficiently high signal-to-noise ratio. Hence, preliminary tests were performed on the ACE instrument using a background source that provided a radiative contrast of about 100 K with the gas in a cell, thereby approximately simulating the atmospheric temperature conditions of the Earth and its atmosphere. Methane, ozone and carbon monoxide gases were used in the cell for the purpose of determining the measurement characteristics of the ACE FTS instrument with respect to the nadir radiation emanating from the planet's surface and atmosphere over most of the thermal infrared region. These measurements were compared with those from the IMG instrument, in order to evaluate if the ACE instrument will have a sufficient signal-to-noise ratio to measure the column amounts of trace gases in the atmosphere. These test measurements were carried out in the Space Laboratory at the University of Toronto, March 12 2003.

For the occultation measurements, the ACE FTS will generally operate at a resolution of 0.02 cm⁻¹; however, to reduce the noise in the nadir observations of the Earth's atmosphere and surface this resolution will be degraded to 0.4 cm⁻¹, or possibly lower, and the measurement time will be extended to 16 s, as summarized in Table 1. This configuration will result in the acquisition of column gas amounts that represent an average measurement over a horizontal spatial scale of about 100 km at the Earth's surface.

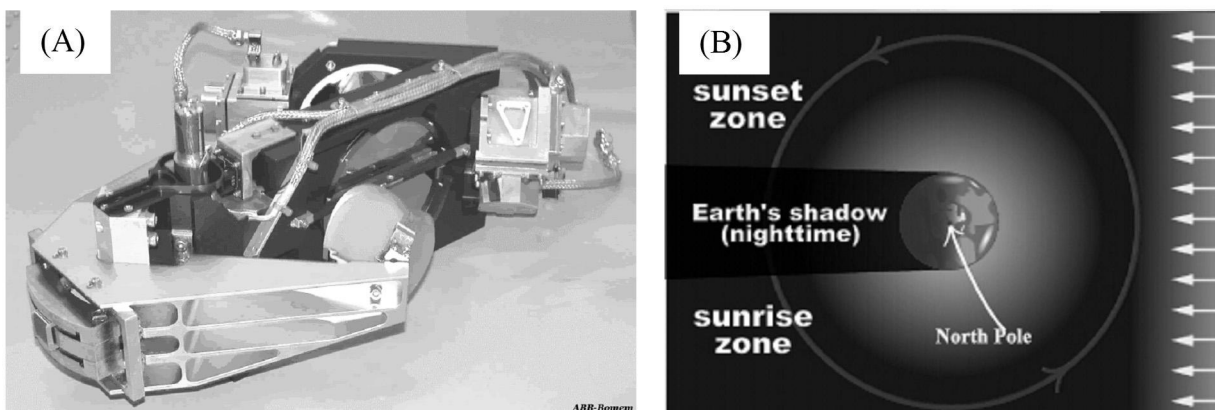


Figure 1: (A) A photograph of the interferometer of the ACE FTS, manufactured by ABB Bomem. (B) The orbit of SCISAT-1, as seen looking down on the Earth's North Pole. For each orbit, the satellite will enter the Earth's shadow, providing the opportunity to measure nadir spectra of the atmosphere.

Table 1: ACE FTS Instrument settings for Occultation and Nadir Measurements

Mode	Resolution (cm ⁻¹)	Single Scan Duration (s)	Total Measurement Duration (s)	Spectral Range (cm ⁻¹)	Footprint (km)
ACE Occultation Measurement (high resolution)	0.02	2	2	700 – 4100	n/a
ACE Nadir Measurement (low resolution)	0.4	0.1	16 (100 scans)	700 – 4100	100 × 1
IMG Nadir Measurement	0.1	10	10 (1 scan)	714 – 3030	8 × 8

2. EXPERIMENTAL PROCEDURE

The ACE FTS instrument is an adapted Michelson interferometer that uses an optimized optical layout. The high-resolution (0.02 cm^{-1}) FTS operates from 2 to 13 microns ($700 - 4100 \text{ cm}^{-1}$) over 2 spectral bands. The first band covers a region ranging from 5.5 to 13 microns (700 to 1800 cm^{-1}) with a Mercury-cadmium-telluride (HgCdTe or MCT) detector, while the second band is from 2 to 5.5 microns (1800 to 4100 cm^{-1}) with an indium antimonide (InSb) detector. The interferometer uses two corner cubes rotating on a center flex pivot to produce the optical path difference (OPD). A folding mirror inside the interferometer is used to increase the OPD.

Normally, a high-temperature 3000 K blackbody was used during the ACE test measurements for the purpose of simulating the occultation scenario. However, in order to reduce the amount of thermal radiation entering the ACE FTS in order to simulate more realistically the nadir scenario, the blackbody temperature was reduced to 1273 K and two attenuators with a transmission of 30% each were added in the optical path, as shown in Figure 2. This configuration had the effect of decreasing the total radiance to the level corresponding to a blackbody at 400 K at 1000 cm^{-1} ; however, the intensity of the Planck function varied significantly at 2000 cm^{-1} from that representing a 400 K source, as illustrated in Figure 3. Here the radiance for the attenuated blackbody is about ten times greater than for a 400 K blackbody.

The gas cell used for the test measurements had a path length of 20 cm and was fitted with ZnSe windows. The gases used for the measurements included methane, ozone and carbon monoxide. The ACE FTS was configured to measure the transmission of the cells using 100 co-additions over a time of 16 s at a resolution of 0.4 cm^{-1} for each gas in the cell. In addition, the spectrum of an empty cell was acquired, as well as a spectrum of a cold blackbody target. The latter was used to characterize the thermal self-emission of the instrument.

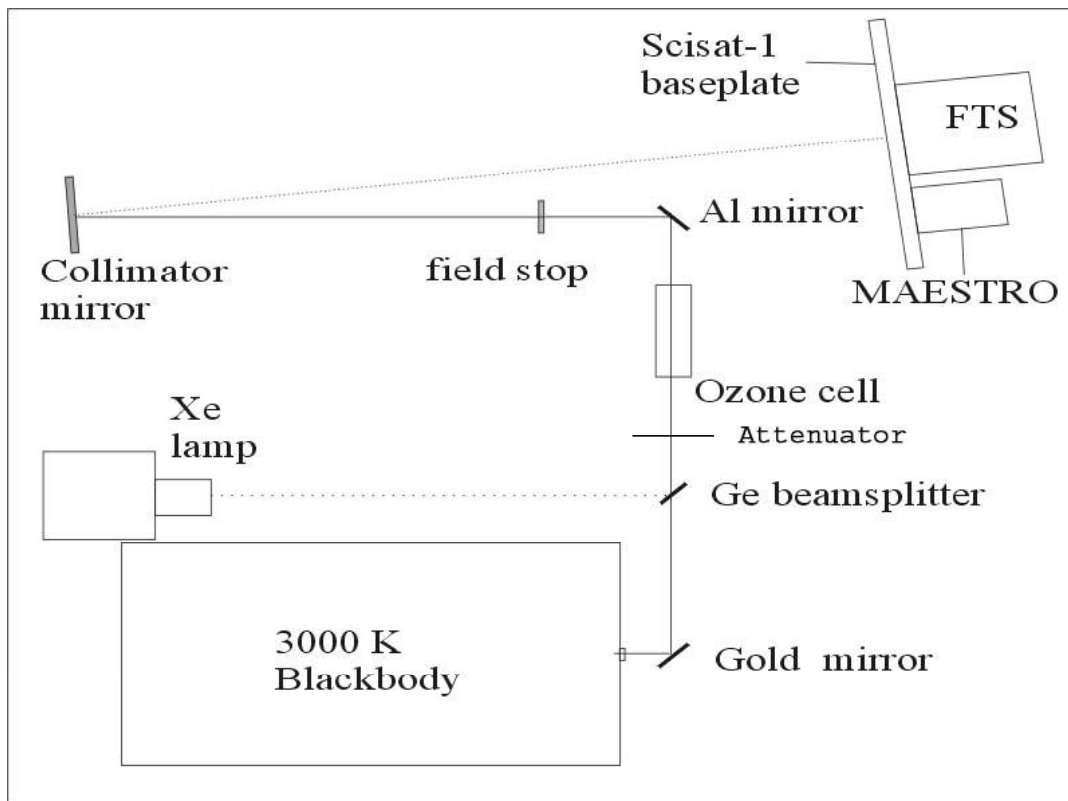


Figure 2: Schematic diagram of the testing configuration used for the nadir measurements with the ACE FTS. The attenuator consisted of two individual meshes each with a transmission of 30%. The blackbody was operated at a temperature of 1273 K.

For comparison purposes, FTS measurements of the cell transmission were also made with a bench model spectrometer (Magna 550, Nicolet Instruments) in order to determine the quantity of gas in the cell. The spectrometer was operated at a resolution of 0.5 cm^{-1} with an MCT detector and a globar source at a temperature of 1500 K. The transmission measurements were first made with the Magna instrument, then by the ACE FTS, and then repeated in the Magna FTS in order to ensure stability of the gas amount in the cell and the reproducibility of the measurement. The high purity methane and carbon monoxide gases were purchased from Matheson Gases.

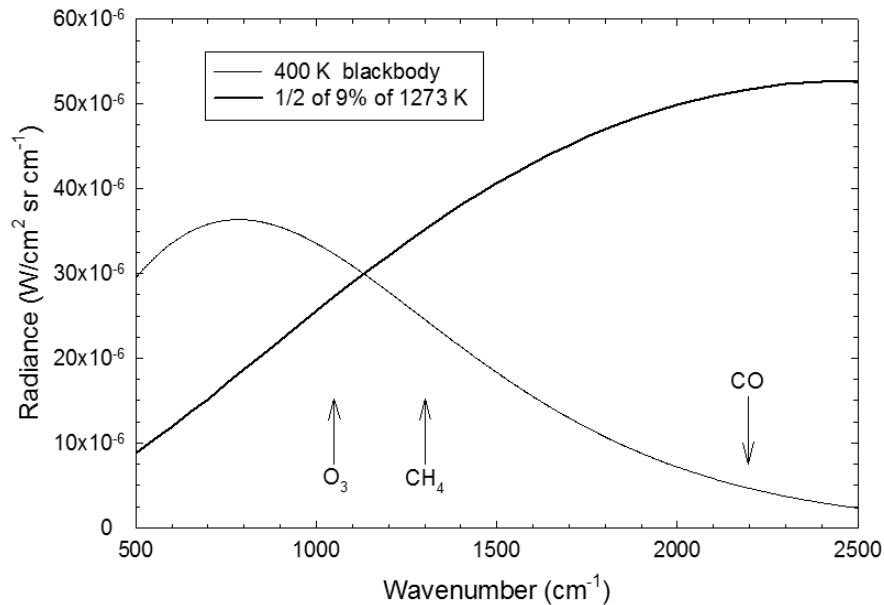


Figure 3: Source intensity for the nadir-testing configuration. A 1273 K blackbody with two attenuators with a transmission of 30% each and a beamsplitter was used to simulate a blackbody at a temperature of 400 K. The intensity of the two curves is in good agreement near 1000 cm^{-1} , where ozone and methane have absorption bands, but diverges by a factor of about ten at 2200 cm^{-1} in the region of CO absorption.

The ozone gas was generated in the cell by a simple and inexpensive approach. The apparatus consisted of the gas cell with a metal electrode inserted through a stopper, which plugged one of the apertures to the cell, as shown in the schematic diagram in Figure 4. The cell was first filled with pure oxygen gas and then a Tesla coil with a typical electrode voltage of about 40,000 V was placed next to the glass wall of the cell near the internal electrode. Atomic oxygen was produced subsequently in the path of the arc inside the cell, which reacted with molecular oxygen in the presence of a third body to form ozone. The process required about 15 minutes of arcing to produce about 150 Dobson units ($1\text{ DU} = 2.73 \times 10^{16}\text{ molecules/cm}^2$) of ozone in the cell, which is about half the amount found in the atmospheric column. The ozone generated in the cell had a time constant of several hours. The background transmission spectrum of the cell was obtained by purging completely with oxygen gas.

An example of an ozone transmission spectrum obtained from the gas cell containing about $6.5 \times 10^{18}\text{ molecules/cm}^2$ (or $\sim 240\text{ DU}$) of ozone is shown in Figure 5. The spectrum was measured at a temperature of 26°C and at a resolution of 0.5 cm^{-1} using the Magna 550 FTIR spectrometer. A simulation of the ozone transmission spectrum using the FASCOD3 transmission model⁷ is also shown for comparison to help identify the ozone absorption bands. The primary absorption by ozone^{8,9} occurs in the $9.6\text{-}\mu\text{m}$ band, and other bands are present at 700, 1700, 2100, 2800 and 3050 cm^{-1} . The absorption features by water vapour and carbon dioxide that are present in the spectrum are due to residual gases, which remain in the desiccated sample compartment of the FTS.

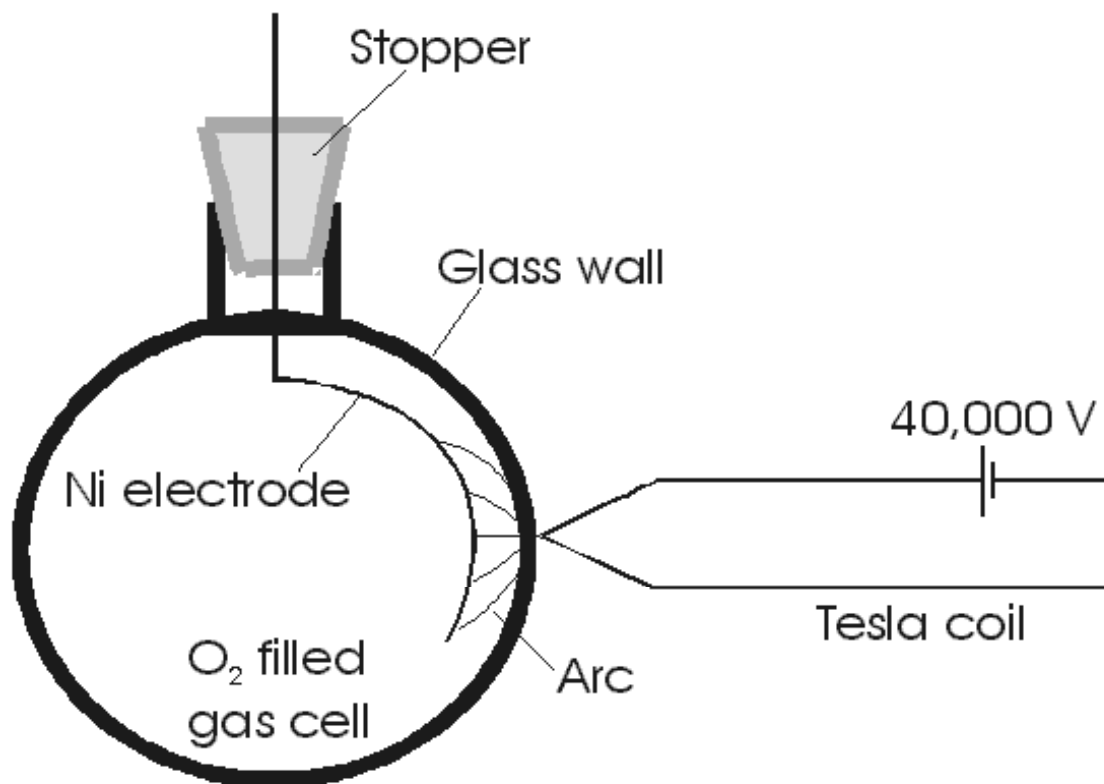


Figure 4: Schematic diagram showing the end-view of the gas cell set up for generating ozone.

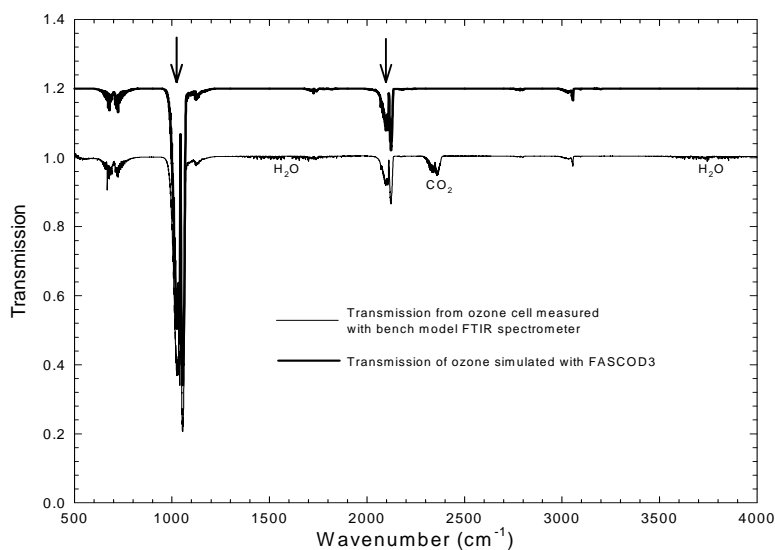


Figure 5: A survey spectrum of the gas cell containing ozone, as measured at a resolution of 0.5 cm⁻¹ using the Magna FTIR spectrometer. The FASCOD3 simulation shows all of the ozone absorption bands in the thermal infrared region. The water and carbon dioxide bands in the measured spectrum are due to residual gases in the sample compartment of the spectrometer. The simulated spectrum has been shifted upwards for clarity. The cell contains about 6.5×10^{18} cm⁻² (~ 240 DU) of ozone.

3. RESULTS AND DISCUSSION

The quantity of methane, ozone and carbon monoxide gases used in the gas cell were roughly equivalent to the column amounts found in the 1976 U.S. standard atmosphere¹⁰. The simulated transmission spectra for these gases are represented in Figure 6. The FASCOD3 transmission model⁷ was used to simulate these nadir transmission spectra for an altitude regime from 40 km to the surface. The line transition parameters incorporated in the FASCOD3 model were from the 2000 HITRAN molecular database¹¹. In addition to the spectra for methane, ozone and carbon monoxide, simulations of the nadir transmission were also performed for carbon dioxide and nitrous oxide to show the possibility for the measurement of these important greenhouse gases. All of the gases in Figure 6 have transmission spectra of the order 50%, and therefore have the potential of being detected with a nadir instrument.

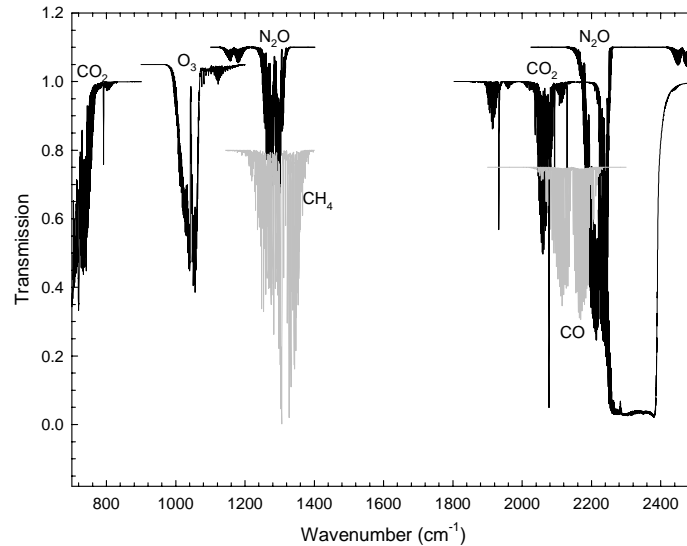


Figure 6: Nadir transmission of several gases simulated with the FASCOD3 model for the 1976 U.S. standard atmosphere. The spectra have been offset to improve the clarity.

An example of the raw test spectrum measured with the ACE FTS is shown in Figure 7. This corresponds to the transmission through a cell of methane using the 1273 K blackbody source attenuated to the approximate level of a 400 K source. The result of the measurement of the empty cell is also shown, as well as the instrument self-emission obtained from a cold target source. The spectra from the cell containing methane and from the empty cell are directly superimposed on each other, except in the region between 1200 – 1400 cm^{-1} where methane absorbs energy. Removing the instrument self-emission contribution and dividing the spectrum of the cell filled with methane by that of the empty cell results in the transmission measurement shown in Figure 8A. The maximum transmission of about 10% is approximately the level that one would find for the U.S. standard atmosphere shown in Figure 6. Also presented in Figure 8A is the transmission result measured with the Magna FTS. The Magna result corresponds to a methane column amount of 1.16×10^{19} molecules/ cm^2 , as determined with the FASCOD3 model. Integrating the two methane bands from the ACE and Magna transmission measurements showed that the ACE measurement gave a result that was 16% smaller. The corresponding column amount derived from the ACE FTS measurement was 9.96×10^{18} molecules/ cm^2 , with the difference attributed to the choice of the location of the baseline. The peak absorptions from the two measurements agree within about 5%. The root-mean-square (rms) noise in the transmission spectrum measured by the ACE FTS is about 0.04 in the 1150 – 1200 cm^{-1} region. However, if the methane band is subdivided into 20 micro-windows between 1250 – 1350 cm^{-1} , then the rms noise is reduced by a factor of 4.5 (or $\sqrt{20}$) yielding an rms signal-to-noise ratio of about 90:1 for methane. This result demonstrates that nadir spectra measured with the ACE FTS should reliably give methane column amounts of the Earth's atmosphere with a precision within about 1%. Figure 8B represents the nadir transmission measured by the IMG spectrometer on the ADEOS satellite. It was measured at a spectral resolution of 0.1 cm^{-1} , and it has a SNR of about 50:1 in the 1150 cm^{-1} region, which is also comparable to the ACE measurement at 0.4 cm^{-1} .

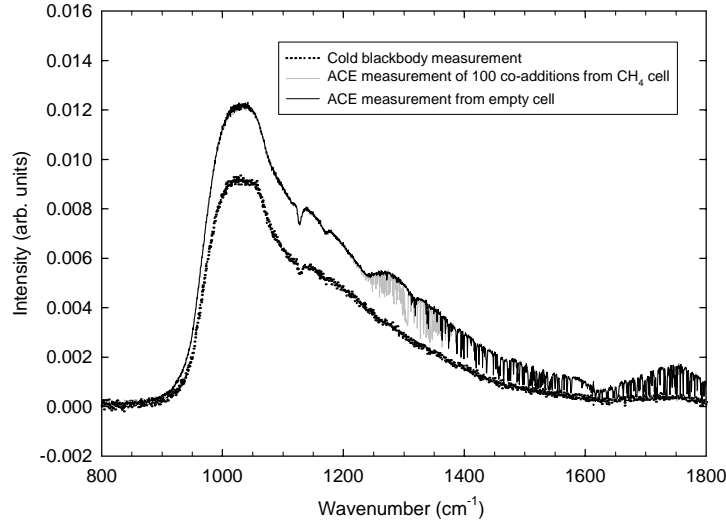
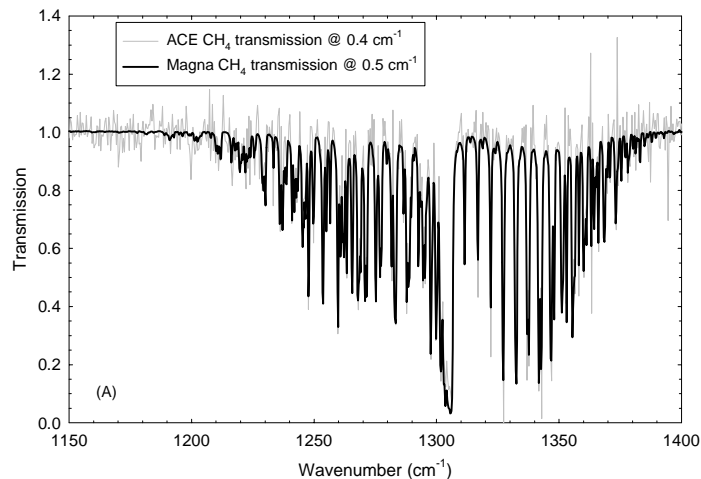


Figure 7: The raw spectra measured with the ACE FTS for the nadir-view configuration. The infrared source consisted of a 1273 K blackbody attenuated by a beamsplitter and two meshes with an overall transmission of 9%.

A similar analysis has been performed for ozone, as shown in Figure 9A, where a comparison is made between the transmission of the ozone absorption bands at 9.6 microns. The transmission spectrum from the Magna result corresponds to an ozone column amount of 3.88×10^{18} molecules/cm², as determined with the FASCOD3 model. Integrating the two ozone bands from the ACE and Magna transmission measurements showed that the ACE measurement was 12% smaller. The corresponding column amount derived from the ACE FTS measurement was 3.47×10^{18} molecules/cm². The peak absorptions from the two measurements agree within about 5%. The rms noise in the transmission spectrum measured by the ACE FTS is about 0.05 in the 1100 – 1150 cm⁻¹ region, resulting in an rms signal-to-noise ratio of about 20:1. By analyzing the band over 20 micro-windows, the signal-to-noise ratio will be increased to about 90:1. Figure 9B represents the nadir transmission measured by the IMG spectrometer. It was measured at a spectral resolution of 0.1 cm⁻¹, and it has a SNR of about 50:1 in the 1100 cm⁻¹ region, which is also comparable to the ACE measurement at 0.4 cm⁻¹. This demonstrates that nadir spectra measured with the ACE FTS should reliably give ozone column amounts of the Earth's atmosphere with a precision of about 1%.



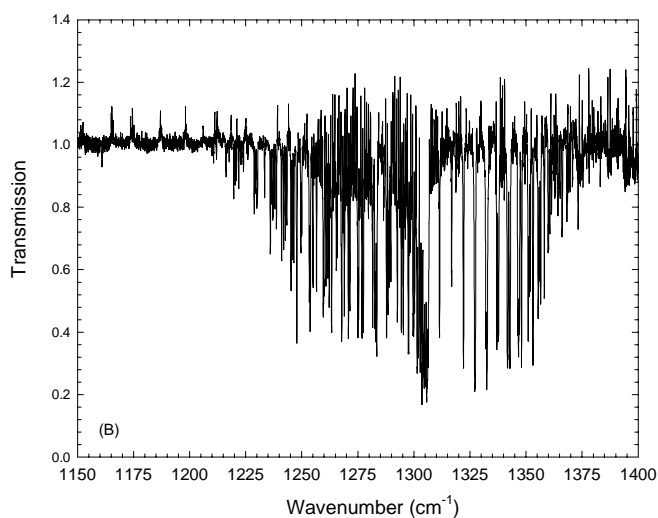
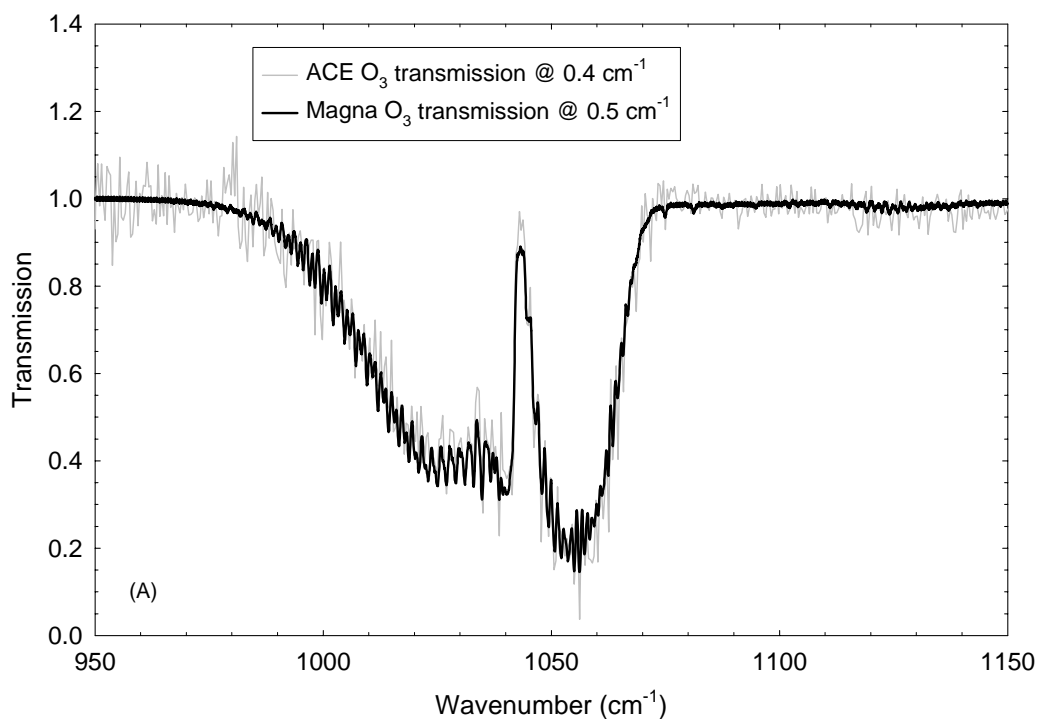


Figure 8: (A) The transmission spectra of methane measured with the ACE and Magna FTS. The methane column amounts derived from the two measurements were 1.16×10^{19} molecules/cm² and 9.96×10^{18} molecules/cm², respectively. (B) The transmission spectrum of methane measured with the IMG instrument at a resolution of 0.1 cm⁻¹. The rms noise was measured to be 50:1 in the 1200 cm⁻¹ region.



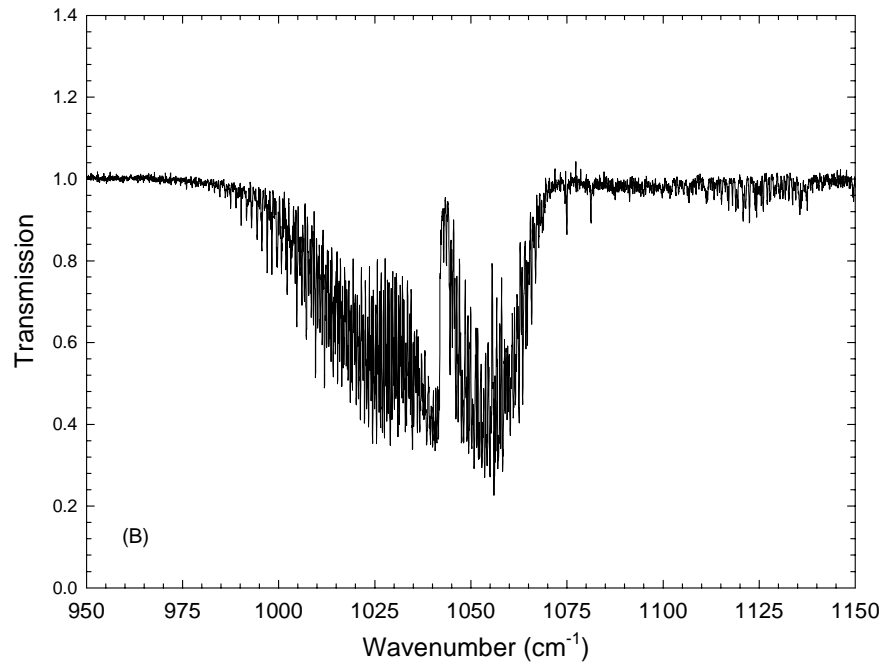


Figure 9: (A) The transmission spectra of ozone measured with the ACE and Magna FTS. The ozone column amounts derived from the two measurements were 3.88×10^{18} molecules/cm² and 3.47×10^{18} molecules/cm², respectively. The measured rms noise is 0.023 (50:1) in the 1100 cm⁻¹ region. (B) The transmission spectrum of ozone measured with the IMG instrument at a resolution of 0.1 cm⁻¹. The rms noise was measured to be 50:1 in the 1100 cm⁻¹ region.

Finally, the analysis performed for carbon monoxide is shown in Figure 10A, where a comparison is made between the transmission of the absorption bands at 2200 cm⁻¹. The transmission spectrum from the Magna result corresponds to a carbon monoxide column amount of 8.68×10^{17} molecules/cm², as determined with the FASCOD3 model. Integrating the two carbon monoxide bands from the ACE and Magna transmission measurements showed that the ACE measurement was 35% smaller. The corresponding column amount derived from the ACE FTS measurement was 5.57×10^{17} molecules/cm². The peak absorptions from the two measurements agree within about 5%. The rms noise in the transmission spectrum measured by the ACE FTS is about 0.016 in the 2000 – 2050 cm⁻¹ region. This is significantly better than the previous results due to the employment of the InSb detector in the band region. This yields an rms signal-to-noise ratio of about 25:1 for carbon monoxide. The analysis of the carbon monoxide absorption throughout 20 micro-windows further increases the signal-to-noise ratio by a factor of 4.5 (or $\sqrt{20}$) to better than 100:1. However, from Figure 3 it is apparent that the source radiance employed in the experiment is about ten times too intense for a 400 K blackbody. Therefore, the signal-to-noise level should be degraded by a factor of ten. In order to be able to retrieve the carbon monoxide column, it may be necessary to degrade the resolution of the spectra by a factor of ten to a value of 4 cm⁻¹, as shown in Figure 10, to compensate for the decrease in signal-to-noise. Even with the resulting decrease in the line absorption at 4 cm⁻¹, it should still be possible to measure the carbon monoxide column with a precision of better than 5%. For comparison, Figure 10B represents the nadir transmission measured by the IMG spectrometer with SNR of about 90:1. The carbon monoxide transmission is lower in the case of the IMG spectrum due to the higher resolution at which the measurement was made.

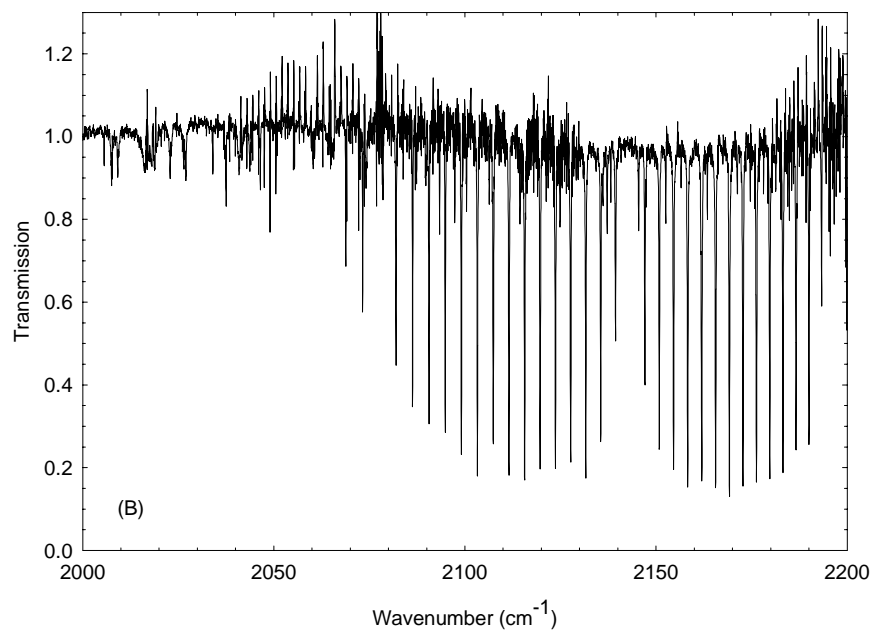
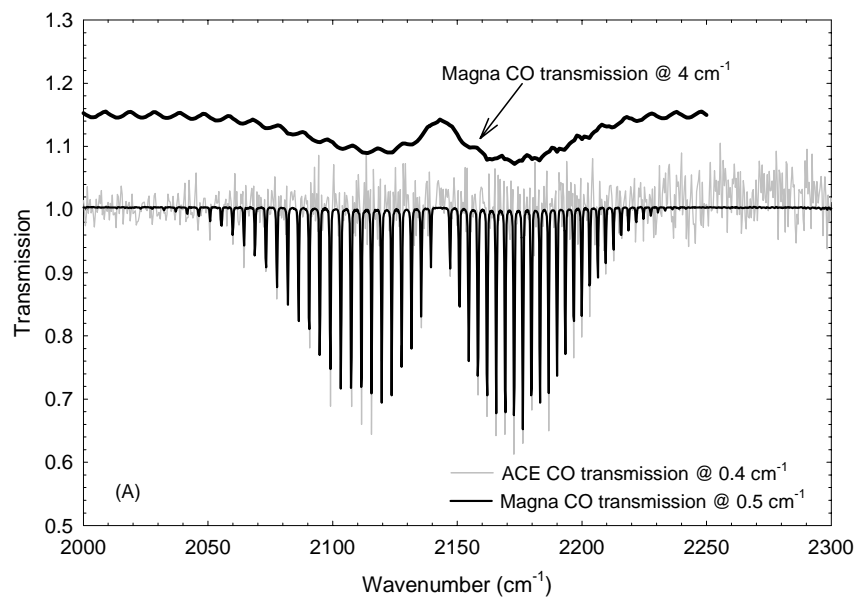


Figure 10: (A) The transmission spectra of carbon monoxide measured with the ACE and Magna FTS. The carbon monoxide column amounts derived from the two measurements were 8.68×10^{17} molecules/cm² and 5.57×10^{17} molecules/cm², respectively. The measured rms noise is 0.014 (75:1). The de-resolved spectrum at 4 cm⁻¹ resolution has been shifted upwards for clarity. (B) The transmission spectrum of carbon monoxide measured with the IMG instrument at a resolution of 0.1 cm⁻¹. The rms noise was measured to be 90:1 in the 2000 cm⁻¹ region.

4. CONCLUSIONS

Transmission measurements of several gases have been measured successfully with the ACE FTS instrument. From a comparison with a standard FTS instrument and the FASCOD3 model, it is apparent that these preliminary measurements show that the retrieval of nadir column amounts should be possible for carbon dioxide, methane, ozone, nitrous oxide and carbon monoxide gases with a typical precision within 5%. In addition, the rms SNR of the ACE measurements are comparable to those measured at a higher spectral resolution of 0.1 cm^{-1} with the IMG instrument onboard the ADEOS satellite. These results are important since they demonstrate that extra science can be acquired from this occultation-viewing instrument, including information on the phenomena of global warming and air pollution, through the measurement of gas column amounts.

ACKNOWLEDGEMENTS

We gratefully acknowledge the generous financial support of Enbridge-Consumers Gas for this work.

REFERENCES

1. S.A. Clough, C.P. Rinsland and P.D. Brown, Retrieval of tropospheric ozone from simulations of nadir spectral radiances from space, *J. Geophys. Res.*, **100**, 16579, 1995.
2. T. Ogawa, H. Shimoda and M. Hayashi, IMG, interferometric measurement of greenhouse gases from space, *Advances in Space Research*, **14**, 25, 1994.
3. W.F.J. Evans and E. Puckrin, The surface radiative forcing of nitric acid for northern mid-latitudes, *Atmospheric Environment*, **35**, 71-77, 2001.
4. IPCC, 2001, Climate Change 2001: The scientific basis. Contribution of working group I to the third assessment report of the Intergovernmental Panel on Climate Change (Houghton, J.T., Y. Ding, D.J. Griggs, M. Noguer, P.J. van der Linden, X. Dai, K. Maskell, and C.A. Johnson (eds.), Cambridge University Press, Cambridge, New York, 2001.
5. Harries, J.E., H.E. Brindley, P.J. Sagoo and R.J. Bantges, Increases in greenhouse forcing inferred from the outgoing longwave radiation spectra of the Earth in 1970 and 1997, *Nature*, **410**, 355-357, 2001.
6. H.G. Reichle, V.S. Connors, J.A. Holland, R.T. Sherrill, H.A. Wallio, J.C. Casas, E.P. Condon, B.B. Gormsen and W. Seiler, The distribution of middle tropospheric carbon monoxide during early October 1984, *J. Geophys. Res.*, **95**, 9845, 1990.
7. S.A. Clough, F.X. Kneizys, G.P. Anderson, E.P. Shettle, J.H. Chetwynd, L.W. Abreu and L.A. Hall "IRS '88: Current Problems in Atmospheric Radiation", J. Lenoble and J.F. Geleyn (eds.), A. Deepak Publishing, 372-375, 1988.
8. J.M. Flaud and R. Bacis, The ozone molecule: infrared and microwave spectroscopy, *Spectrochimica Acta A*, **54**, 3-16, 1998.
9. S.N. Mikhailenko, A. Barbe, J.J. Plateaux and V.G. Tyuterev, New analysis of $2\nu_1 + \nu_2$, $\nu_1 + \nu_2 + \nu_3$, and $\nu_2 + 2\nu_3$ bands of ozone in the 2600-2900 cm^{-1} region, *J. Mol. Spectrosc.*, **196**, 93-101, 1999.
10. G.P. Anderson, S.A. Clough, F.X. Kneizys, J.H. Chetwynd, and E.P. Shettle, 1986: AFGL Atmospheric Constituent Profiles (0-120 km), AFGL-TR-86-0110, Optical Physics Div., Air Force Geophysics Laboratory, Hanscom AFB, MA.
11. L.S. Rothman, A. Barbe, D. Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, K. Yoshino, The HITRAN molecular spectroscopic database: edition of 2000 including updates through 2001, *Journal of Quantitative Spectroscopy and Radiative Transfer*, **82**, in press, 2003.