Calibration of instruments for atmospheric ozone measurements II: the ACE FTS and MAESTRO spectrograph

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ABSTRACT

A novel and simple technique is described for the calibration of satellite instruments for the measurement of atmospheric ozone. Ozone is generated in a gas cell and spectral measurements of the ozone absorption are measured with a standard Fourier-transform spectrometer (FTS) in order to determine the amount of ozone in the cell. The satellite instrument then views the cell using an appropriate illumination source. In this presentation the preliminary results from the ozone calibration procedure are presented for the ACE FTS and MAESTRO instruments to show how consistently both instruments measure ozone. The thermal infrared band of ozone at 4.7 microns was used to provide the calibration of the ACE interferometer, whereas the Chappuis band at 600 nm was used to characterize the response of the MAESTRO instrument. The ozone transmission spectra that were derived from the ACE FTS and MAESTRO spectrograph measurements were found to be in good agreement with the simulated spectra of known amounts of ozone from a radiative transfer model. All of the results yielded column ozone amounts that were within 10% of each other. These calibration measurements were taken at the University of Toronto in March 2003, before the expected launch date of the SciSat-1 satellite in August 2003.

Keywords: satellite remote sensing, occultation, FTIR, ozone, calibration

1. INTRODUCTION

The SciSat-1 satellite is expected to be launched in August 2003 carrying the Atmospheric Chemistry Experiment. It consists primarily of two science instruments, the ACE Fourier-transform spectrometer (FTS) and an optical spectrograph for the Measurement of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation (MAESTRO). SCISAT-1 will use the occultation of the Sun by the Earth to make detailed determinations of the chemical and dynamical processes that control the distribution of ozone in the stratosphere and upper troposphere in heights ranging from 4 to 100 kilometres above the Earth's surface. In particular, there will be a strong focus placed on measurements taken of the Arctic winter stratosphere. The satellite will orbit the Earth 15 times each day providing an opportunity to observe sunlight that has passed through the Earth's atmosphere during 15 brief 'sunrises' and 'sunsets', resulting in 30 sets of observations each day.

The FTS and MAESTRO instruments will all share a single suntracker and will have approximately the same field of view. Therefore, it is important to characterize the response of the ACE FTS and the MAESTRO instruments to ozone in order to ensure that they each give consistent results[1,2]. To this end we have employed a simple and novel method for calibrating the ACE FTS and MAESTRO instruments for ozone. The ozone is generated in a gas cell and a bench model FTS is used to quantify the ozone amount in the cell. Subsequent measurements of the cell are then made with the SciSat-1 instruments to determine their preliminary measurement response to the ozone, and to verify that the two instruments give self-consistent results.

This work was performed March 12, 2003 at the University of Toronto. The calibration procedure has been successfully applied previously to the OSIRIS spectrograph onboard the ODIN satellite[3].

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2. EXPERIMENTAL PROCEDURE

The ACE FTS instrument is an adapted Michelson interferometer using an optimized optical layout. The high-resolution (0.02 cm^{-1}) FTS operates from 2 to 13 microns (700 – 4100 cm^{-1}) over 2 spectral bands. The first band covers a region ranging from 5.5 to 13 microns (700 – 1800 cm^{-1}) with a Mercury-cadmium-telluride (HgCdTe or MCT) detector, while the second band is from 2 to 5.5 microns (1800 – 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.

MAESTRO is a dual optical spectrometer that will cover the 0.285 to 1.03 micron spectral region. It will use two spectrographs (280 - 550 nm, 500 - 1030 nm) to improve the stray light performance. The spectral resolution is about 1 – 2 nm and the detectors are linear photodiode arrays with 1024 elements. The design is based on a simple concave grating with no moving parts. The entrance slit will be held horizontal to the horizon during sunrise and sunset by controlling the spacecraft roll with a startracker and a momentum wheel on the satellite bus. The FTS and MAESTRO instruments will all share a single suntracker and will have approximately the same field of view. The vertical resolution of MAESTRO, however, will be about 1 km and will have a signal-to-noise ratio in excess of 1000. It will measure primarily ozone, nitrogen dioxide and aerosol/cloud extinction. The optical configuration for the ozone test measurements with the SciSat-1 instruments at the University of Toronto is shown in Figure 1.

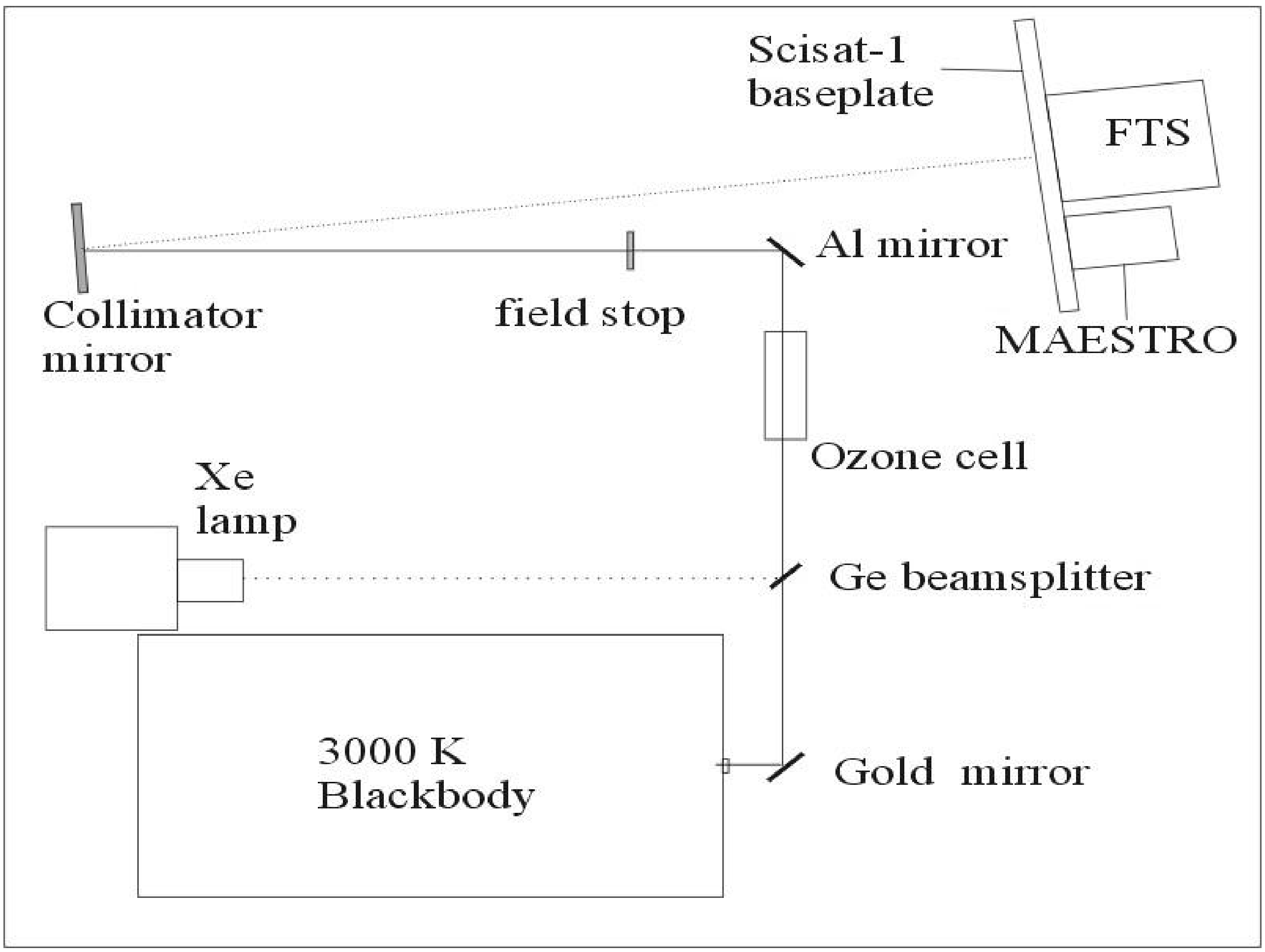

Figure 1: Schematic diagram of the testing configuration used for the ozone measurements with the ACE FTS and MAESTRO instruments. The germanium beamsplitter serves to combine the ultraviolet light of the xenon source with the visible light of the high-temperature blackbody radiator.

The ozone gas was generated in the cell by a simple and inexpensive approach. The apparatus consisted of a Pyrex gas cell with a path of 20 cm, and a metal electrode inserted through a stopper, which plugged one of the apertures to the cell, as shown in the schematic diagram in Figure 2. 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 by the reaction,

$$O + O_2 + O_2 \Leftrightarrow O_3 + O_2 \tag{1}$$

The process required about 15 minutes of arcing to produce about 150 Dobson units (1 DU = 2.73×10^{16} 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.

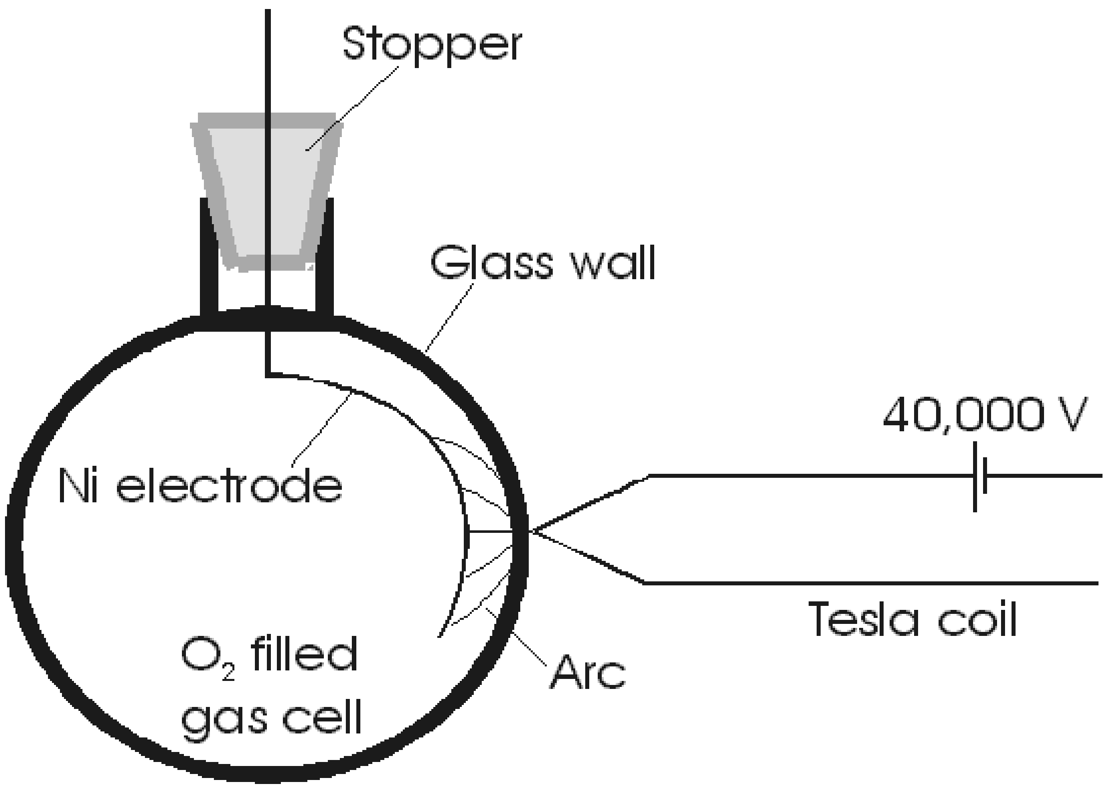

Figure 2: Schematic diagram showing the end-view of the gas cell set up for generating ozone.

For comparison purposes, FTS measurements of the cell transmission were 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 combination of the ACE FTS and MAESTRO instruments. The measurements were then repeated with the Magna FTS in order to verify the amount of ozone degradation that occurred during the time needed for the SciSat-1 measurements. The entire measurement process required about one hour.

3. RESULTS AND DISCUSSION

An example of an ozone transmission spectrum obtained from the gas cell containing about 6.5×10^{18} molecules/cm^2 (or ~ 240 DU) of ozone is shown in Figure 3. 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 model[4] is also shown for comparison to help identify the ozone absorption bands.

The primary absorption by ozone[5,6] occurs in the 9.6-μm 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.

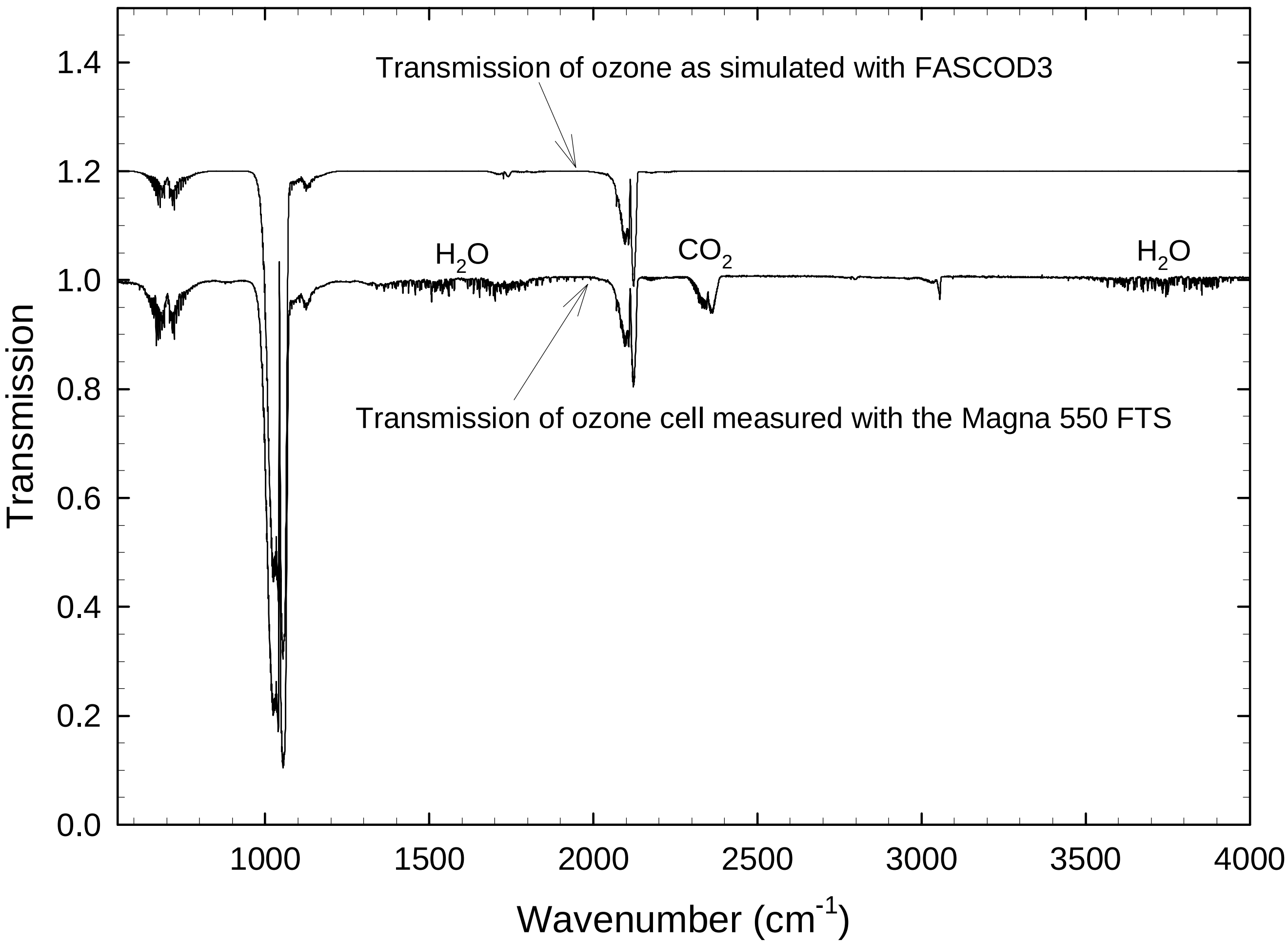

Figure 3: A survey spectrum of the gas cell containing ozone, as measured at a resolution of 0.5 cm^{-1} using the Magna FTIR spectrometer. The FASCOD3 simulation shows all of the ozone absorption bands in the thermal infrared region. The water and carbon dioxide bands in the measured spectrum are due 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.

In order to determine the amount of ozone that is present in the cell, the FASCOD3 model was used to simulate the ozone absorption in the 2100 cm^{-1} region over a path length of 20 cm. The ozone line transition parameters were taken from the 2000 HITRAN molecular database[7]. The ozone amount in the simulation was altered until the band integrals of the measurement and simulation were in agreement over the 2000 – 2150

cm^{-1} region. Figure 4A shows the comparison of the measured ozone band and one simulated with FASCOD3. By comparing the band integrals, it was found that an ozone column amount of 6.95×10^{18} molecules/cm^2 (~ 260 DU) was present in the cell. This is a little less than the amount of about 300 DU that is present in the full atmospheric column. This measurement corresponds to the ozone amount that was present in the gas cell before it was moved into the clean room and analysed by the ACE FTS and MAESTRO instruments.

Due to the slow degradation of ozone in the cell, it was necessary to use the Magna FTS to re-measure the amount after the analysis by the SciSat-1 instruments was completed. This result is represented by Figure 4B, where it is shown that the ozone amount in the cell decreased by about 20% to a value of 5.36×10^{18} molecules/cm^2 (~ 200 DU) over a period of about one hour. Normally during past calibration experiments with other instruments we have found that the ozone amount typically decays by just 2 or 3% over several hours. Hence, it is apparent that our cell had a small leak, which did not significantly affect the outcome of the experiment. Due to the limited time nature involved in the ACE calibration, it was not possible to find the leak and seal the cell completely.

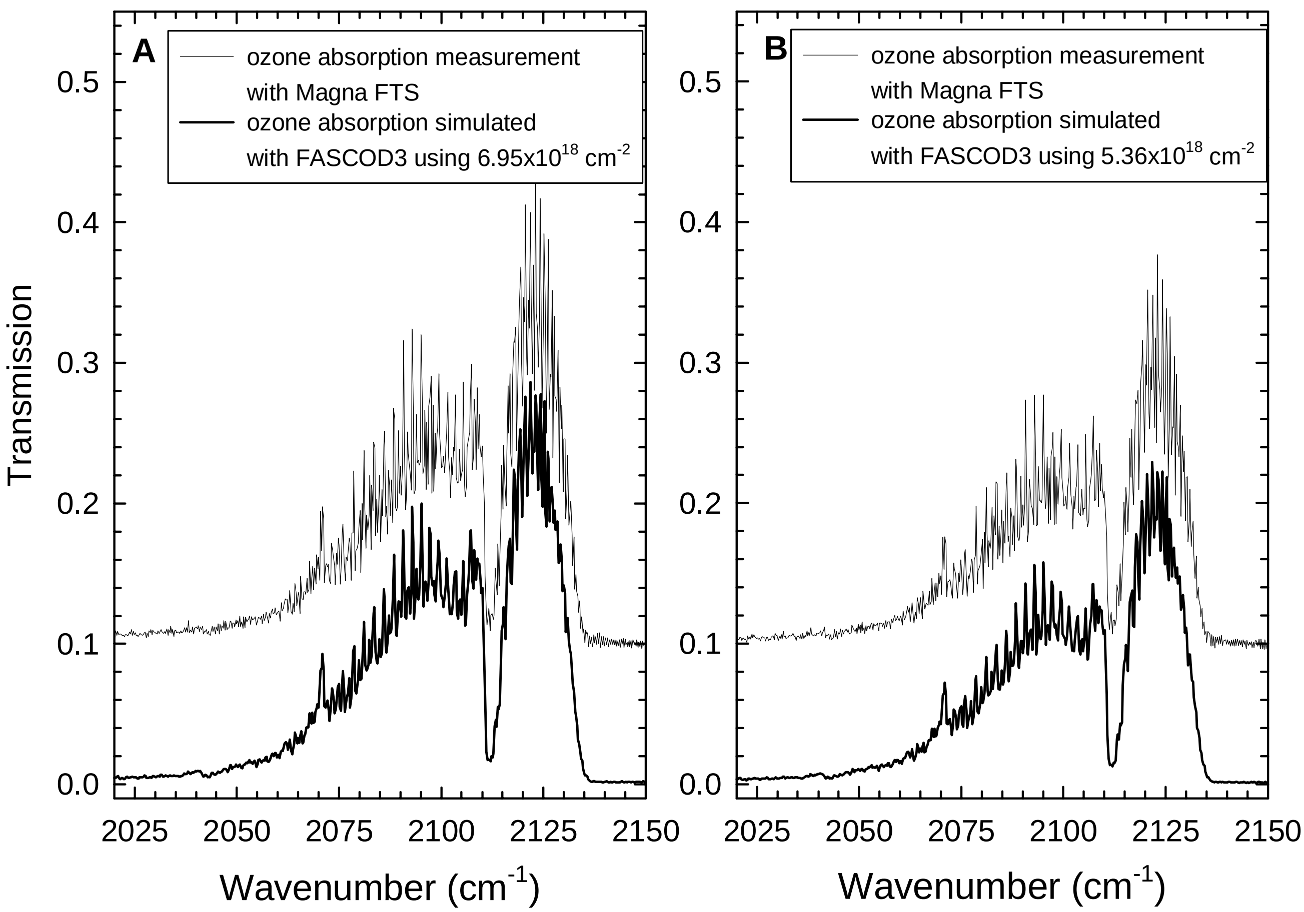

Figure 4: Determination of the ozone amount in a gas cell with FTIR spectroscopy. (A) The comparison of the band integrals for the measurement and the FASCOD3 simulation shows that 260 DU (6.95×10^{18} molecules/cm^2) of ozone was present in the gas cell. This evaluation was made before the ozone cell was analysed with the ACE FTS and MAESTRO instruments. (B) The same ozone cell analysed after being measured with the ACE and MAESTRO instruments. The quantity of ozone in the cell was degraded by 20% to an amount of 200 DU (5.36×10^{18} molecules/cm^2) over a period of about 1 hr.

The corresponding transmission measurement of the ozone cell made by the ACE FTS is shown in Figure 5. The measurement was made at a resolution of 0.02 cm^{-1} for the two bands at 9.6 and 4.7 microns. In order to determine the quantity of ozone in the cell as measured with the ACE FTS, the resolution was degraded to 0.5 cm^{-1}, as shown in Figure 5, to increase the signal-to-noise of the transmission result.

As in the earlier process for determining the ozone amount with the Magna FTS, the FASCOD3 model was used to simulate the ozone absorption in the 2100 cm^{-1} region over a path length of 20 cm. The ozone amount in the simulation was increased until the band integrals of the measurement and simulation were in agreement over the 2000 – 2150 cm^{-1} region, as shown in Figure 6. It was found that an ozone column amount of 5.42×10^{18} molecules/cm^2 (~ 200 DU), was present in the cell as determined by the ACE FTS. This compares well (within ~ 10%) with the ozone column amount of 6.16×10^{18} molecules/cm^2 that was determined from the average of the 'before' and 'after' measurements made with the Magna FTS.

The corresponding transmission spectrum obtained with the MAESTRO spectrograph in the visible region is shown in Figure 7. Ozone absorbs in the Chappuis band in the 600 nm region and below 350 nm in the Huggins band[8]; however, the light source did not provide a sufficient level of light below 400 nm to measure the latter band. Also included in the figure is the simulated result of the Chappuis band transmission that corresponds to an ozone amount of 6.16×10^{18} molecules/cm^2, that is, the average amount determined by using the thermal transmission spectra measured with the Magna FTS. The simulation was performed with the MODTRAN4 band model[9]. The agreement between the MAESTRO measurement and the simulation is excellent, as indicated by the difference of 8% between the two Chappuis absorption bands. This demonstrates that the MAESTRO instrument is capable of making calibrated ozone measurements of the atmosphere that are consistent with the ozone column amount determined with the laboratory FTS.

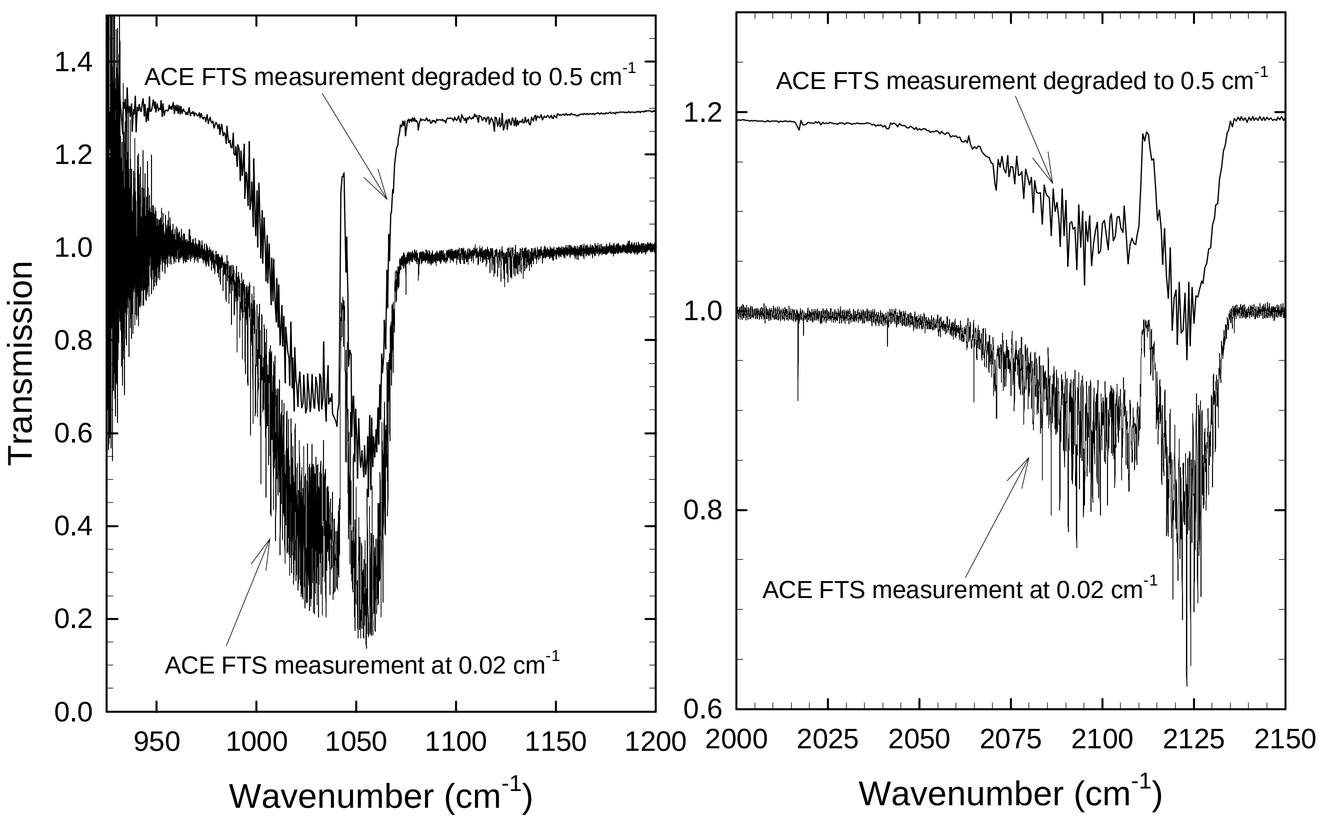

Figure 5: The transmission spectra of the ozone gas cell measured with the ACE FTS at a high resolution of 0.02 cm^{-1}. Also shown are the spectra degraded to a resolution of 0.5 cm^{-1} for the purpose of determining the column amount of ozone in the cell (see Figure 6).

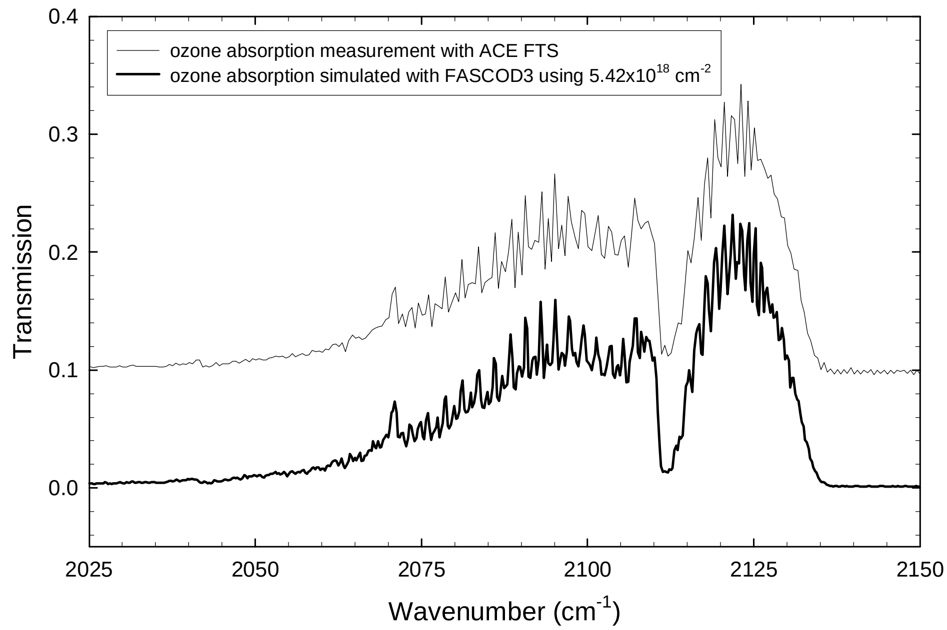

Figure 6: The transmission spectra of ozone as measured with the ACE FTS and simulated with the FASCOD3 model. The comparison of the band integrals for the measurement and simulation shows that 200 DU (5.42×10^{18} molecules/cm^2) of ozone was present in the gas cell. This evaluation compares favourably with the average result of 6.16×10^{18} cm^{-2} that was determined from the measurements made with the Magna FTS.

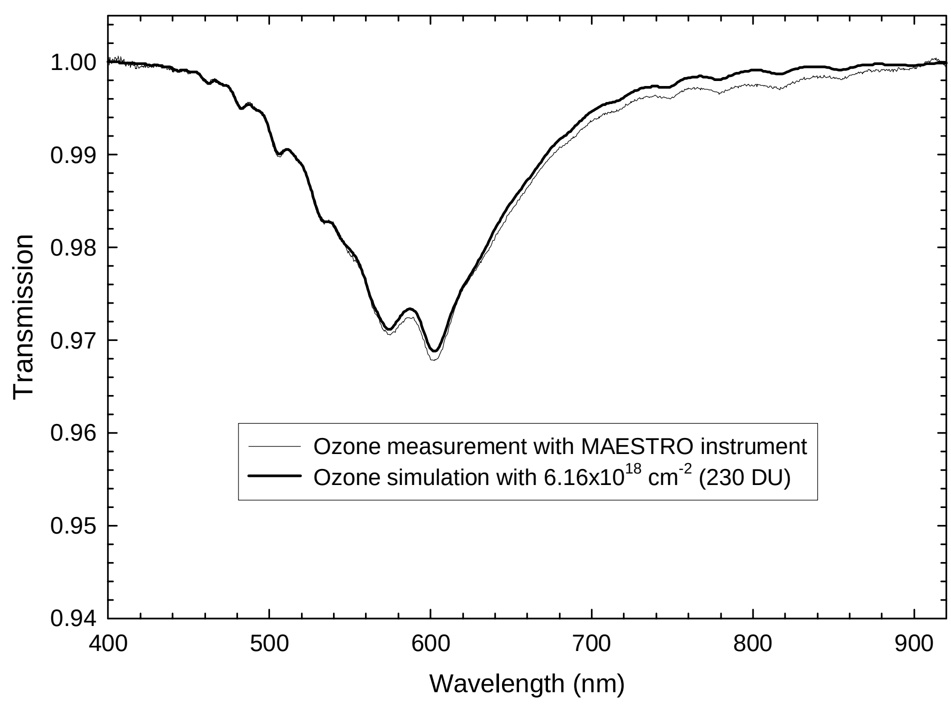

Figure 7: The transmission spectra of ozone measured with the MAESTRO instrument and simulated with the MODTRAN4 model. An amount of 6.16×10^{18} cm^{-2} of ozone was used in the simulation. This was based on the ozone amount determined from the average of the Magna FTS results.

4. CONCLUSIONS

A novel and simple technique is described for the calibration of measurements of atmospheric ozone by the ACE FTS and MAESTRO instruments on the SciSat-1 satellite. Ozone was generated in a gas cell and spectral measurements of the ozone absorption were measured with a standard FTIR in order to determine the amount of ozone in the cell. The satellite instruments then viewed the same cell using a high-temperature blackbody or ultraviolet illumination source. The preliminary ozone transmission spectra that were derived from the ACE FTS and MAESTRO spectrograph measurements were found to be in good agreement with the simulated spectra of known amounts of ozone as determined by the radiative transfer models FASCOD3 and MODTRAN4.

It is recommended that all future satellite instruments for measuring ozone be calibrated during pre-flight using this or a similar technique. Ground-based ozone-monitoring instruments, such as Brewer or Dobson spectrophotometers, that are used for validating satellite instruments should also be calibrated using this portable and inexpensive technique.

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REFERENCES

1. WMO (World Meteorological Organization), Scientific assessment of ozone depletion: 1998, *Global Ozone Research and Monitoring Project – Report No. 44, World Meteorological Organization*, Geneva, 1999.

2. SPARC-IOC-GAW Assessment of Trends in the Vertical Distribution of Ozone, *SPARC report No.1, WMO Global Ozone Research and Monitoring Project Report No. 43*, 1998.

3. E. Puckrin and W.F.J. Evans, "The calibration of instruments for atmospheric ozone measurement with a sealed ozone cell: the OSIRIS/ODIN spectrograph", *Advances in Space Research*, in press, 2003.

4. 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.

5. J.M. Flaud and R. Bacis, The ozone molecule: infrared and microwave spectroscopy, *Spectrochimica Acta A*, **54**, 3-16, 1998.

6. S.N. Mikhailenko, A. Barbe, J.J. Plateaux and V.G. Tyuterev, New analysis of 2ν1+ ν2, ν1+ ν2+ν3, and ν2+2ν3 bands of ozone in the 2600-2900cm-1 region, *J. Mol. Spectrosc.*, **196**, 93-101, 1999.

7. 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.

8. J.P. Burrows, A. Richter, A. Dehn et al., Atmospheric remote-sensing reference data from GOME – 2. Temperature-dependent absorption cross sections of O_3 in the 231-794 nm range, *J. Quant. Spectrosc. Radiat. Transfer*, **61**, 509-517, 1999.

9. L.W. Abreu, F.X. Kneizys, G.P. Anderson et al., MODTRAN, *The Proceedings of 1991Battlefield Atmospherics Conference*, El Paso, Texas, 1991.