

# Spectroscopy From Orbit

Peter Bernath

**THE MISSION:** To improve understanding of the chemical and dynamical processes that control ozone distribution in the upper troposphere and stratosphere.

**THE APPROACH:** To make comprehensive simultaneous measurements of trace gases, thin clouds, aerosols and temperature by solar occultation from a small satellite.

**A**nthropogenic changes in atmospheric ozone have led to an increased amount of ultraviolet radiation reaching the ground and may affect climate.<sup>1</sup> For more than a quarter century, atmospheric chemists have vigorously pursued a better understanding of the mechanisms by which chemical pollutants damage Earth's ozone layer. Canada's Earth-orbiting Atmospheric Chemistry Experiment (ACE) mission is the latest space-based effort to explore ozone depletion, with a special focus on changes occurring over Canada and the Arctic that could be damaging to sensitive northern plant and animal life.

Launched for the Canadian Space Agency (CSA) by the National

Aeronautics and Space Administration (NASA) on August 12, 2003, the ACE mission is the first in CSA's Science Satellite (SCISAT) program. A high-inclination (74°), circular, low-Earth orbit (650 km) enables the ACE mission instruments to cover the tropical, mid-latitude and polar regions (Fig. 1).

## Instrumentation

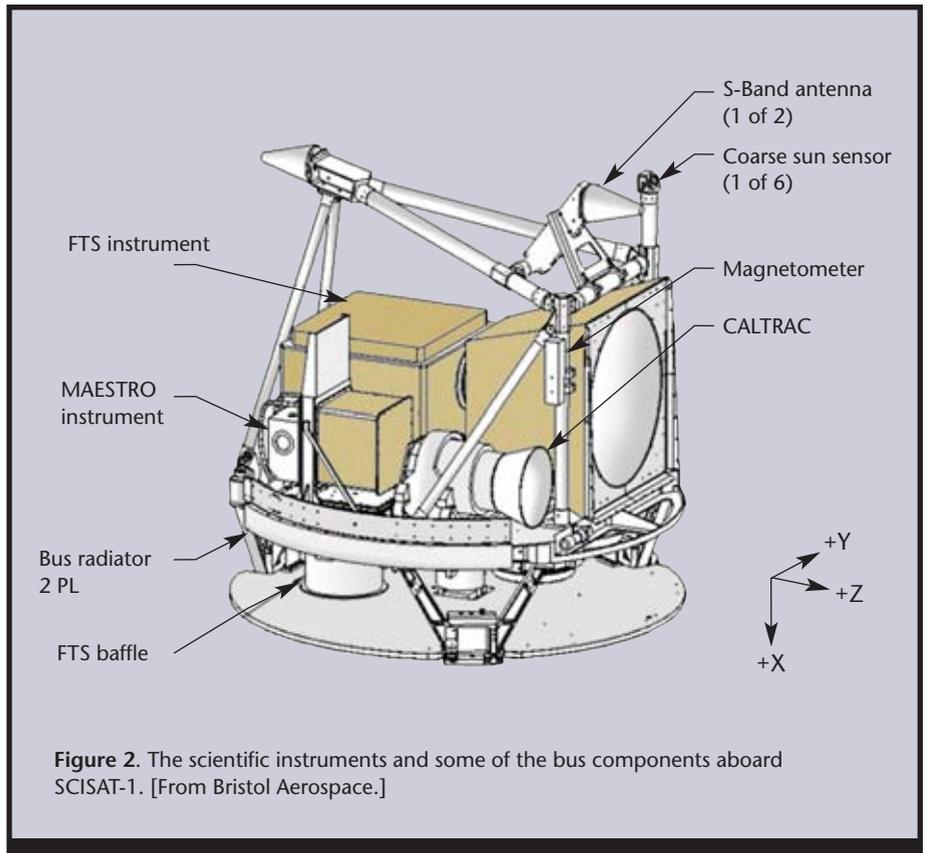
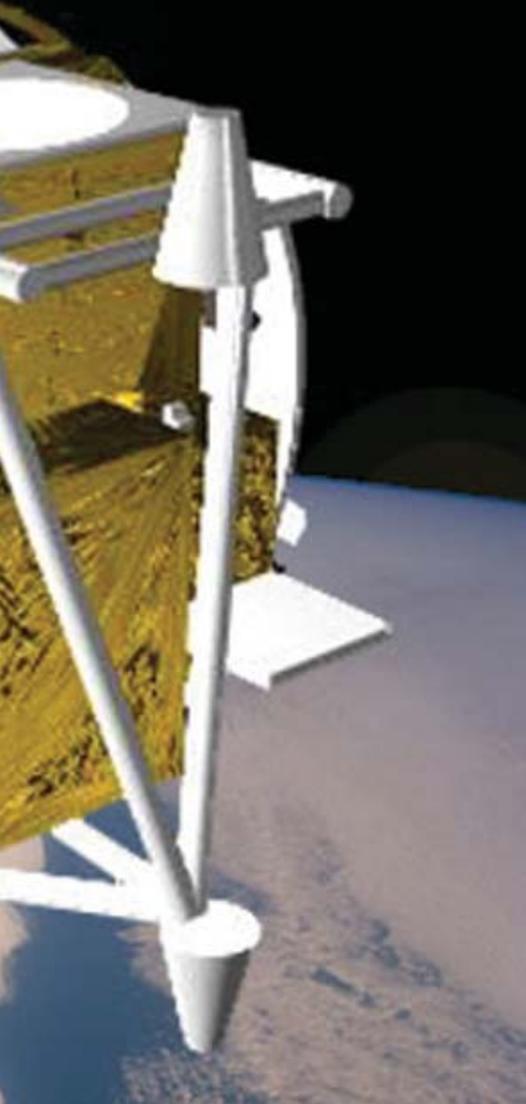
A high-resolution ( $0.02\text{ cm}^{-1}$ ) infrared Fourier transform spectrometer (FTS) operating from  $2\text{--}13\ \mu\text{m}$  ( $750\text{--}4400\text{ cm}^{-1}$ ) measures the vertical distribution of trace gases and temperature. During sunrise and sunset, the FTS measures infrared absorption spectra in the limb direction that contain information from different

atmospheric layers and are inverted to provide vertical profiles of atmospheric constituents.

The vertical resolution is about 4 km from the cloud tops to about 150 km. Aerosols and clouds are being monitored using the extinction of solar radiation at  $1.02$  and  $0.525\ \mu\text{m}$ , as measured by two filtered imagers. The ACE-FTS and imagers were built by ABB-Bomem in Quebec City, and the satellite bus—the part of the satellite that is not instruments—was made by Bristol Aerospace in Winnipeg (Fig. 2).

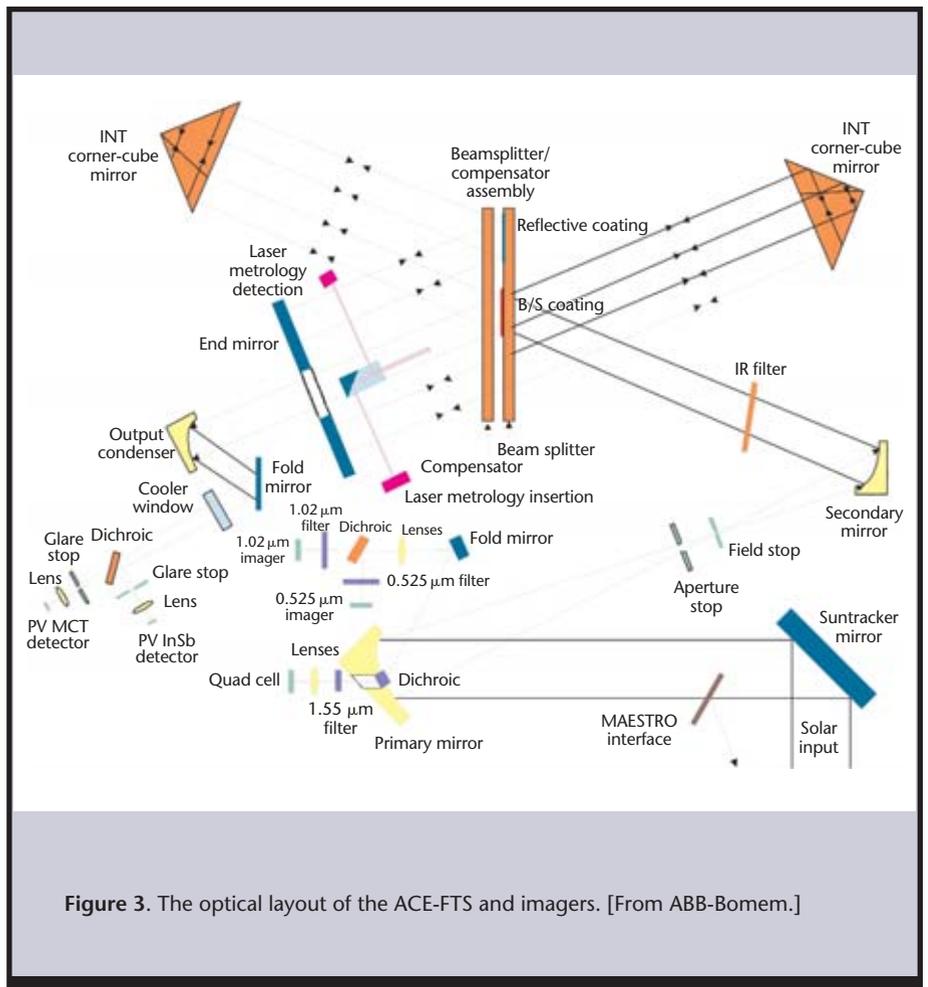
A second instrument, Measurement of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation (MAESTRO), also orbits on

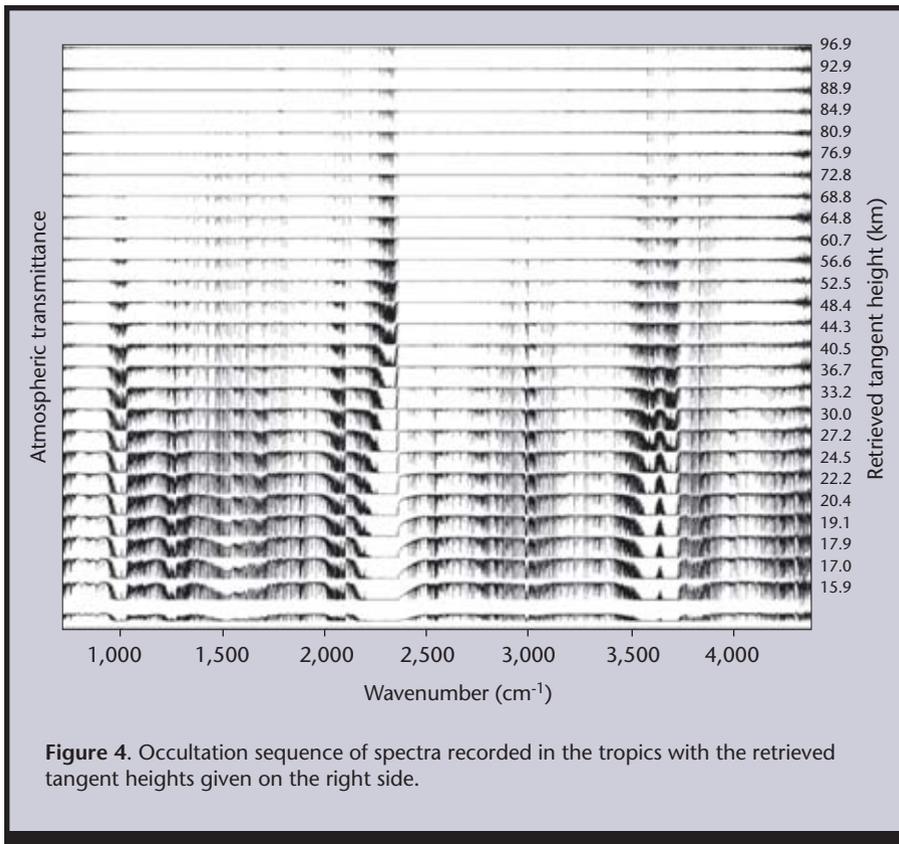
**Figure 1.** ACE satellite recording atmospheric spectra during sunrise. [From Bristol Aerospace.]



SCISAT-1, for which C. T. McElroy of the Meteorological Service of Canada (MSC) serves as the principal investigator. MAESTRO, a dual optical spectrograph, covers the 285–1,030 nm spectral region. It has a vertical resolution of 1–2 km and measures primarily ozone, nitrogen dioxide and aerosol/cloud extinction. A collaborative group of scientists from MSC, the University of Toronto and EMS Technologies in Ottawa designed and built MAESTRO.

The main ACE instrument (Fig. 3) is a custom-designed Michelson interferometer. It uses two corner cubes rotating on a central flex pivot (not shown) to produce the optical path difference. An end mirror inside the interferometer





**Figure 4.** Occultation sequence of spectra recorded in the tropics with the retrieved tangent heights given on the right side.

enables it to double pass the radiation, and thus to increase the optical path difference.

The ACE design fully compensates for tilt and shear of both moving and stationary optics inside the interferometer. The optical position is measured with interference fringes obtained with a diode laser operating at 1,500 nm. The instrument is also equipped with a visible imager and a near-infrared imager. A pointing mirror, controlled by a suntracker servo-loop, locks on the sun and tracks it while the instruments take measurements.

Double-sided interferograms are Fourier transformed on the ground to obtain the desired atmospheric spectra. The FTS covers the 750–4,400  $\text{cm}^{-1}$  range using two detectors (InSb and HgCdTe). A passive radiator pointing toward deep space cools the detectors to less than 100 K (typically 80–90 K).

The visible/near-infrared imager has two filtered channels at 0.525 and 1.02  $\mu\text{m}$ , chosen to match two of the wavelengths monitored by the Stratospheric Aerosol and Gas Experiment

(SAGE II) instrument,<sup>2</sup> launched in 1984 aboard NASA's Earth Radiation Budget Satellite. These two wavelengths are useful for studying clouds and aerosols because they are relatively free of absorption by atmospheric molecules.

The detectors in the imagers are  $256 \times 256$  active pixel sensors (binned to  $128 \times 128$ ) provided by FillFactory, based in Mechelen, Belgium. The total field of view of the imagers is 30 mrad, to be compared to the 9 mrad angular size of the solar image is greater than 1,000.

MAESTRO is a small (about 8 kg) spectrograph designed to cover the 285–1,030 nm region in two overlapping pieces. The use of two spectrographs (280–550 nm, 500–1,030 nm) improves the stray-light performance and permits simultaneous measurements of the two bands at a moderate spectral resolution of about 1–2 nm, depending on wavelength.

The detectors are linear EG & G Reticon photodiode arrays with 1,024 elements. The design is based on a simple concave grating with no moving parts.

The entrance slit is held horizontal to the horizon during sunrise and sunset by controlling the spacecraft roll. The FTS, imagers and MAESTRO all share a single suntracker and have approximately the same direction of view. The vertical resolution of MAESTRO is 1–2 km and the signal-to-noise ratio exceeds 1,000.

### SCISAT-1

CSA received the original ACE proposal in January 1998 and the agency selected the experiment for flight in November of the same year. Final integration of the instruments with the SCISAT-1 bus occurred at CSA's David Florida Laboratory near Ottawa, Ontario, during May 2003. The satellite was then shipped to Vandenberg Air Force Base for integration with a Pegasus XL rocket built by Orbital Sciences of Dulles, Va.

Launch occurred in the early evening of August 12, 2003, by dropping the rocket from the bottom of a Lockheed L-1011 jumbo jet a short distance off the coast of California. The launch and early-orbit phase proceeded without difficulty.

The spacecraft recorded its first atmospheric spectra in early November 2003 and the scientific team found that the FTS produced excellent spectra with a signal-to-noise ratio in excess of 300 over most of the spectral band. Only at the edges of the band (below about 900  $\text{cm}^{-1}$  and above 3,700  $\text{cm}^{-1}$ ) does the signal-to-noise ratio drop below 100. CSA declared SCISAT-1's scientific activities fully operational on February 17, 2004.

SCISAT-1 orbits Earth 15 times a day. The measurement sequence that occurs during a sunset occultation starts with the suntracker pointing to deep space to record a set of instrument self-emission spectra. The deep-space spectra are followed by a set of high sun reference spectra obtained by pointing to the center of the sun, followed by a sequence of occultation spectra recorded as the sun sets through the atmosphere (Fig. 4). The atmospheric spectra and high sun spectra are corrected for instrument self-emission before computation of the transmission spectra.

The ACE mission is based on the successful (but now-retired) Atmospheric Trace Molecule Spectroscopy (ATMOS) instrument, which flew four times on

NASA's Space Shuttle.<sup>3</sup> ATMOS recorded some remarkable high resolution solar occultation spectra. The miniaturized ACE-FTS instrument has about one-tenth the mass, power and volume of ATMOS.

### Data processing

Raw ACE data are transmitted from space to two Canadian ground stations and transferred using the Internet from CSA's Mission Operations Centre in St. Hubert to the Science Operations Centre at the University of Waterloo in Ontario. At Waterloo, the data are archived and transformed into data products for distribution to members of the science team.

In the case of the FTS, the Science Operations Center transforms the raw interferograms (level 0) into corrected atmospheric spectra (level 1) using software supplied by the instrument contractor, ABB-Bomem. Level 2 data—the height profiles of the volume mixing ratios of atmospheric constituents—are generated by analysis software developed at the University of Waterloo. During the level 1 to level 2 data processing, spectra measured during an occultation (Fig. 4) are used to infer variations as a function of altitude for the atmospheric quantities of interest.

Prior information about meteorological quantities (pressure and temperature) is not sufficiently accurate for quantitative analysis of the ACE-FTS measurements. Therefore, the first step in level 1 to level 2 data processing requires the retrieval of the temperature and pressure profiles for each occultation. Retrievals of temperature from the FTS data assume a fixed CO<sub>2</sub> volume-mixing ratio in the altitude range of about 10–70 km. In essence, the relative CO<sub>2</sub> line intensities determine the temperature and the absolute line intensities give the pressure.

The second step in level 1 to level 2 data processing involves the retrieval of altitude profiles of the gaseous atmospheric constituents. For the FTS data, the temperature profile is held constant and selected microwindows are used to retrieve the altitude profiles using a "global fit" approach.<sup>4</sup> Figure 5 provides an example of such a retrieval for ozone.

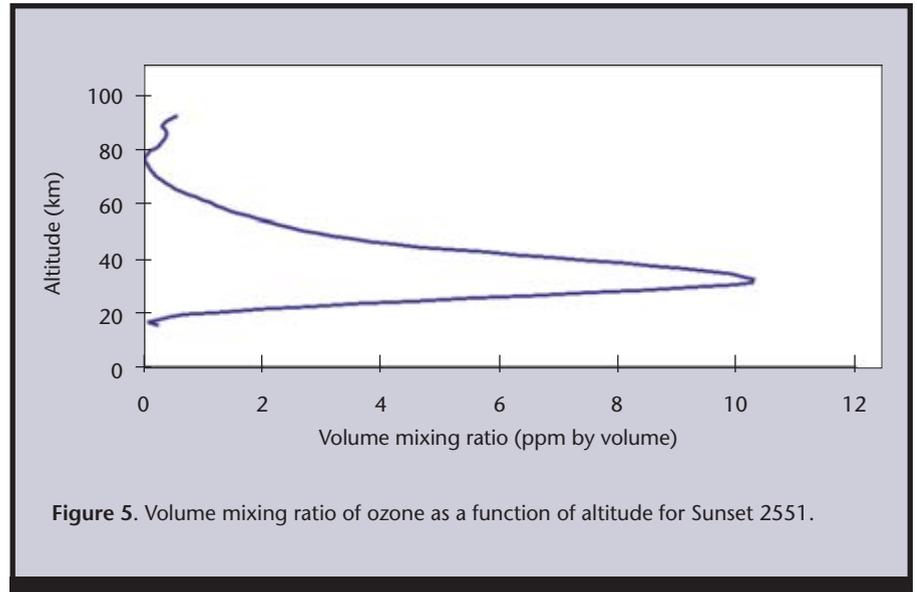


Figure 5. Volume mixing ratio of ozone as a function of altitude for Sunset 2551.

Note that Fig. 4 and Fig. 5 are based on the data of a single tropical occultation recorded on February 2, 2004, 4:21 Universal Time at 9° S latitude 132° W longitude over the Pacific Ocean.

The ACE mission is completely dependent on the availability of spectroscopic data for the required retrievals of atmospheric molecules and temperature. We have adopted the HITRAN 2004 spectroscopic database for the line parameters and cross sections for the initial processing of ACE-FTS data.<sup>5</sup>

The University of Waterloo has generated version 1.0 of the ACE-FTS level 2 data, which consists of profiles of 18 molecules: H<sub>2</sub>O, O<sub>3</sub>, N<sub>2</sub>O, CO, CH<sub>4</sub>, NO, NO<sub>2</sub>, HNO<sub>3</sub>, HF, HCl, N<sub>2</sub>O<sub>5</sub>, ClONO<sub>2</sub>, CCl<sub>2</sub>F<sub>2</sub>, CCl<sub>3</sub>F, COF<sub>2</sub>, CHF<sub>2</sub>Cl, HDO, SF<sub>6</sub>, plus *p* and *T*, interpolated on a 1-km grid for sunrises from February through October 2004. Although version 1.0 is intended primarily for validation exercises, researchers will also use it for preliminary scientific investigations.

These studies include a look at the current levels of stratospheric water vapor and trends of various molecules through comparison with the previous ATMOS measurements. Spring 2004 in the northern hemisphere saw a major enhancement of NO and NO<sub>2</sub> levels in the stratosphere, possibly as a result of strong auroral events in the fall 2003. ACE captured this enhancement, and we are investigating this effect in some

detail. The ACE-FTS also recorded the first infrared spectra of polar mesospheric clouds in summer 2004.<sup>6</sup>

### Acknowledgments

We thank the ACE team of scientists, engineers and managers whose efforts have made the mission a success. Thanks also to ABB-Bomem (M. A. Soucy) for permission to reproduce Fig. 3, and to Bristol Aerospace (T. Doherty and I. Walkty) for permission to use Figs. 1 and 2. Funding for ACE is provided by the Canadian Space Agency and the Natural Sciences and Engineering Research (NSERC) of Canada, and additional funding is provided by the NSERC-Bomem-CSA-MSI Industrial Research Chair in Fourier Transform Spectroscopy. We also are grateful for the launch and other support provided by NASA.

Peter Bernath (bernath@uwaterloo.ca) is a professor of chemistry and physics at the University of Waterloo in Ontario, and the mission scientist for ACE.

### References

1. D. I. Wardle et al., eds., *Ozone Science: A Canadian Perspective on the Changing Ozone Layer*, Environment Canada (1997).
2. L. E. Mauldin et al., *Opt. Eng.* **24**, 307 (1985).
3. M. R. Gunson et al., *Geophys. Res. Lett.* **23**, 2333 (1996).
4. M. Carlotti, *Appl. Opt.* **27**, 3250 (1988).
5. L. S. Rothman et al., *J. Quant. Spectrosc. Rad. Transfer*, in press (2005).
6. P. F. Bernath et al., *Geophys. Res. Lett.*, in press (2005).