Journal of Quantitative Spectroscopy & Radiative Transfer 148 (2014) 18–21

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

ACE infrared spectral atlases of the Earth's atmosphere

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ARTICLE INFO

Article history:
Received 3 April 2014
Received in revised form
20 June 2014
Accepted 22 June 2014
Available online 28 June 2014

Keywords:
High resolution atmospheric spectra
Infrared
Fourier transform spectrometer
Atmospheric Chemistry Experiment (ACE)
satellite

ABSTRACT

Five infrared atmospheric atlases are presented using solar occultation spectra from the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS) in low earth orbit. The spectral atlases were created for Arctic summer, Arctic winter, mid-latitude summer, mid-latitude winter and the tropics. Each covers the spectral range from 700 to 4400 cm^{-1} and consists of 31 spectra that span an altitude range of 6–126 km in 4-km altitude intervals. To improve the signal-to-noise ratio, each spectrum in the atlas is an average of at least several hundred individual ACE-FTS limb transmission spectra. Representative plots in pdf format at 10 km (troposphere), 30 km (stratosphere), 70 km (mesosphere), and 110 km (lower thermosphere) are also available.

1. Introduction

Spectra of the Earth's atmosphere are the basis for remote sensing of composition and physical properties. Spectra can be measured from the ground, from a variety of air-borne platforms including balloons, and from orbit. Often atmospheric spectroscopy cannot be avoided; for example, scientists observing the Earth's surface from orbit or making astronomical observations from the surface all have to peer through the atmosphere and make "atmospheric corrections" to their data, e.g. [1].

The atmosphere is largely transparent in the visible and microwave regions, but atmospheric molecules absorb strongly in the infrared spectral domain. The infrared is therefore often the best region to make atmospheric observations and at the same time the most difficult and complex to analyze. Not surprisingly there is a considerable history of high resolution infrared spectroscopy of the atmosphere. Observations are typically made in absorption using the sun as a source of radiation [2] but they can also be made in thermal emission by the MIPAS [3] and TES instruments [4].

From the ground, there is a comprehensive set of high resolution solar observations made with the Fourier transform spectrometer (FTS) associated with McMath–Pierce Solar Telescope at Kitt Peak [5]. Such solar spectra inevitably contain a mixture of atmospheric and solar lines that can be separated (to some extent) using the Langley method, i.e., atmospheric lines vary with solar zenith angle and solar lines do not, e.g. [6]. Other notable ground-based spectra include the atmospheric atlas prepared by Meier et al. based on observations made at Kiruna, Sweden [7], the Jungfraujoch solar atlases [8,9] and the University of Denver atlases [10]. The University of Denver atlases [10] are notable because they include line assignments. There are also international networks such as Network for the Detection of Atmospheric Composition Change (NDACC, http://www.ndsc.ncep.noaa.gov/) and Total Column Carbon Observing Network (TCCON, http://www.tccon.caltech.edu/) that rely on high resolution infrared spectroscopy to monitor the state of the atmosphere.

High resolution solar spectra have also been recorded from high altitude balloons, for example by the University

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http://dx.doi.org/10.1016/j.jqsrt.2014.06.016

of Denver FTS [10], the MkIV FTS [11], and from orbit by the ATMOS [12] and ACE [2] FTSs. It is only from the orbit that it is possible to record pure solar spectra and pure atmospheric spectra. The pioneering ATMOS instrument flew on NASA's Space Shuttle in 1985, 1992, 1993 and 1994 and resulted in two solar atlases [13,14] and one atmospheric atlas [15]. The ATMOS solar atlas also includes line identifications [16]. The ACE instrument was launched in August 2003 and has been recording spectra since February 2004. Although a very high signal-to-noise ACE atlas of the solar spectrum has been produced [17] (including line identifications), no representative set of atmospheric spectra have been published yet.

Representative atmospheric spectra with high signal-to-noise ratios are useful for the identification and study of trace constituents. They can be used to test atmospheric transmission models and spectroscopic databases such as HITRAN [18]. With the discovery of hundreds of exoplanets, these spectra also find application in the prediction of the spectra of earth-like exoplanets. The technique of transit or transmission spectroscopy, which measures the depth of primary exoplanet transit dips as a function of wavelength, has the same geometry as the occultation technique used by ACE and ATMOS [19,20].

2. Description of the ACE-FTS spectra

SCISAT was launched by NASA on August 12, 2003 into a circular low Earth orbit at an inclination of 74° and altitude of 650 km. This orbital geometry provides coverage of tropical, mid-latitude and polar regions (about 85°N to 85°S). The ACE mission was originally designed for only two years but has maintained functionality for more than ten years with only minor problems. During this time the ACE-FTS has taken 62,000 measurements of the atmosphere by solar occultation, i.e., using a limb-viewing geometry during sunrise and sunset. Each measurement is a series of atmospheric absorption spectra from 5 km (in the absence of clouds) to 150 km tangent altitude using the sun as a light source [2].

The ACE-FTS is a high-resolution (0.02 cm^{-1}) Fourier transform spectrometer operating from about 750 to 4400 cm^{-1} in the infrared region. The maximum optical path difference is ± 25 cm and the internal field of view is 6.25 mrad; no apodization is applied to the routine ACE spectra. The ACE-FTS uses two photovoltaic detectors (InSb and HgCdTe) with a dichroic element splitting at 1810 cm^{-1} to maintain the same field of view. The external field of view (FOV) is circular with an angular diameter of 1.25 mrad, which corresponds to a vertical resolution of about 4 km on the limb. It can take up to 30 measurements per day except for approximately 3 weeks in June and again in December when no atmospheric measurements are possible from the ACE orbit [2].

During an occultation a spectral scan is taken every 2 s and the entire spectral range is covered in each single scan. The total measurement time for sunrise or sunset changes over the orbital cycle so more atmospheric spectra can be taken at certain times of the year, and less at others. Each occultation consists of 27–65 atmospheric spectra due to the changing measurement time.

3. Construction of mean ACE-FTS spectra

To create the seasonal atlases, occultations were chosen based on season and latitude. The occultations were divided into five atlas groups with similar atmospheric conditions: Arctic summer, Arctic winter, mid-latitude summer, mid-latitude winter and tropics. Summer occultations were obtained within the months of June, July and August; winter occultations were obtained in December, January and February. All occultations used in creating the atlases were in the northern hemisphere except occultations in the tropical atlas group. Table 1 shows the time period and latitudes for each atlas group. Any occultations that were inside or on the edge of the polar vortex were removed from the average. To determine whether an occultation is inside or on the edge of the polar vortex, the derived meteorological products were used [21] for an altitude range of 15–28 km.

Spectra were divided into 4-km bins from 4 km to 128 km and then averaged to create an average atmospheric profile. One spectrum was created for each 4 km bin of data. At each altitude, the spectrum label was taken as the midpoint between the upper and lower limit of the bin (e.g., 8–12 km bin is labeled as 10 km). Typically about 800 spectra were added together and the continuum signal-to-noise ratio is about 8000. Fig. 1 shows the signal-to-noise ratio (SNR) of a typical occultation measured by the ACE-FTS. The SNR in the averaged spectra varies with wavenumber, and will be some constant factor larger than the “local” value at a particular wavenumber in Fig. 1, because SNR increases approximately proportional to the square root of the number of spectra included in the average. For example, if 800 spectra went into the average, you would multiply the curve in Fig. 1 by roughly 28.2 (the square root of 800). At high altitudes, the atmospheric lines were under-resolved so exhibit the characteristic sin $(x)/x$ lineshape function of the FTS. To smooth this ringing, Norton–Beer strong apodization was applied and then a calibration factor was used to match HITRAN line positions for CO_2 [18]. The peaks in the average spectrum were

Table 1
Time period and latitudes for each atlas group.

Atlas group	Time period	Latitude
Arctic summer	*Months*: June, July, August 2006–Jun to 2008–Aug	60°N–90°N
Arctic winter	*Months*: December, January, February 2004–Dec to 2008–Feb	60°N–90°N
Mid-latitude summer	*Months*: June, July, August 2006–Jun to 2008–Aug	30°N–60°N
Mid-latitude winter	*Months*: December, January, February 2004–Dec to 2008–Feb	30°N–60°N
Tropical	*All months*: 2004–Apr to 2008–Aug	30°N–30°S

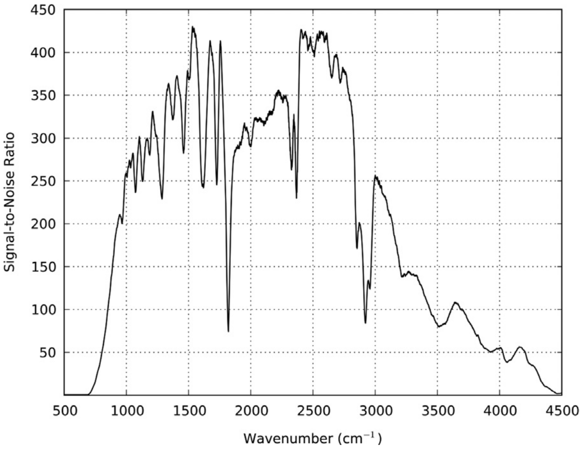

Fig. 1. Signal-to-noise ratio of a typical occultation from 2012.

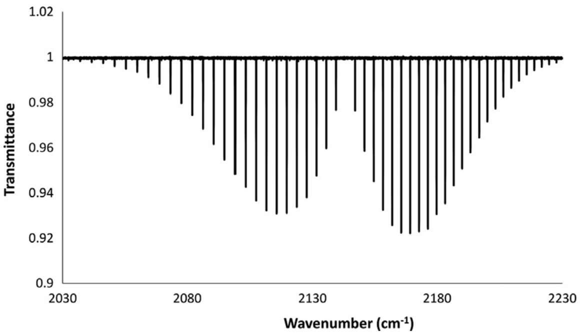

Fig. 2. 1–0 CO absorption band for the 104–108 km bin from the tropical averages.

found using the Bruker OPUS program and then a factor was calculated using up to 50 strong CO_2 lines between 2300 and 2390 cm^{-1} between 98 and 118 km. For each 4 km bin (98–102, 102–106, 106–110, 110–114, 114–118) a calibration factor was obtained and then averaged together for these bins to determine a single factor applied to all spectra in each atlas.

4. Description of the ACE-FTS atmospheric atlases

Five atmospheric atlases (mid-latitude summer, mid-latitude winter, Arctic summer, Arctic winter, and tropics) have been prepared using averaged ACE-FTS spectra. Each atlas consists of a set of 31 individual spectra from 6 km to 126 km.

The very high SNR reveals significant spectral detail in the averaged spectra. Fig. 2 shows the 1–0 CO band for the 104–108 km bin from the tropical averages. The peak absorption depth for the strongest lines is less than 10 percent, yet the noise on the baseline is barely visible on this scale. In fact, weak lines from subsidiary CO isotopologues can be seen between the strong CO main isotopologue lines.

Fig. 3 shows the averaged spectra for an HCl line from a number of bins in the tropical averages. The peak absorption in the 64–68 km bin for this line is about 1.5 percent. In a single ACE-FTS measurement, this would be just above the noise level at the given wavenumber, and so the upper altitude limit for HCl retrievals from the ACE-FTS would be in the 64–68 km altitude range. In the averaged spectra, however, the HCl line is clearly visible up to the 76–80 km altitude bin.

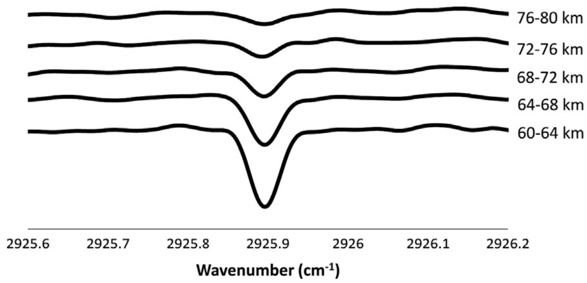

Fig. 3. An HCl line for five altitude bins from the tropical averages. The baseline for each plot is offset for clarity. The peak absorption depth for the line from 64 to 68 km bin is roughly 1.5 percent.

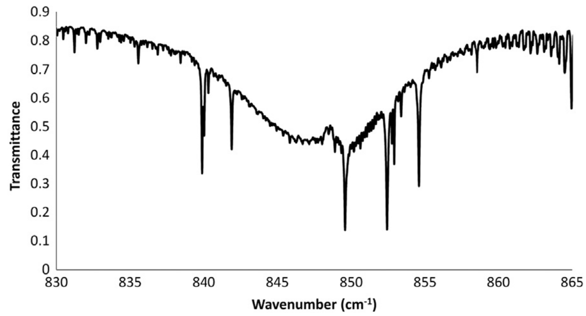

Fig. 4. A portion of the spectrum for the 8–12 km bin from the tropical averages containing a broad absorption feature from CFC-11.

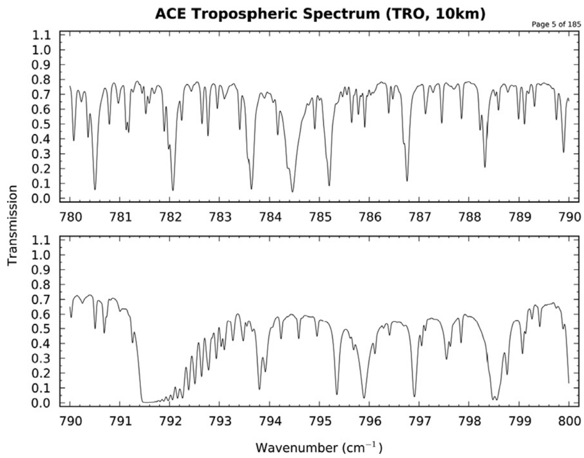

Fig. 5. A representative page from the tropical atlas for the 8–12 km bin.

Note that the atmospheric spectra get increasingly “cluttered” as you move to lower altitude, with more lines and more molecules providing significant contributions to the spectra. In the troposphere, in addition to the relatively sharp gas-phase lines, there are a number of heavier molecules with broad absorption features in the spectra. Fig. 4 shows a spectral region in the 8–12 km bin from the tropical averages that contain a strong CFC-11 absorption feature, the broad “dip” in the apparent baseline.

Spectra for each atlas are given in ASCII format with one file per spectrum. Each of the five atlas sets has a table of details (ASCII format) that provides information generated from the average. These tables are provided as an on-line supplement. The table lists the number of spectra used in each average spectrum, the average pressure, temperature, tangent height and density for each altitude. The atmospheric atlases have also been created in portable document format (PDF) for each profile at 4 different altitudes: 10 km, 30 km, 70 km, and 110 km to give a representative display transmission spectra for the upper troposphere, mid stratosphere, mesosphere and lower thermosphere, respectively. All spectra and files are also available at the ACE web site http://www.ace.uwaterloo.ca/atlas.html. A representative page from the tropical atlas for the 8–12 km bin is given in Fig. 5.

Acknowledgments

The ACE mission is supported primarily by the Canadian Space Agency. Some support was also provided by the NASA Planetary Atmospheres Program. We thank S.D. McLeod for assistance in preparing the atlases.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.jqsrt.2014.06.016.

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