

TRACE CONSTITUENTS MEASUREMENTS DEDUCED FROM SPECTROMETRIC OBSERVATIONS ON-BOARD SPACELAB

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ABSTRACT

The observation of infrared absorption lines by means of a grille spectrometer on board Spacelab 1 allows the determination of CO₂ and CO in the low thermosphere and in the middle atmosphere. Equal abundances of CO and CO₂ are found at 115 ± 5 km altitude. CO₂ is observed to depart from its homospheric volume mixing ratio near 100 km, dropping by a factor of 10, 15 km higher. The CO largest number density is observed near 70 km altitude, close to the H Lyman alpha photoproduction peak.

The analysis of one run dedicated to the observation of water vapor shows a middle atmospheric mixing ratio of this species within the limits : 3 to 8 ppmv up to 70 km altitude, with the indication of an increase from 30 to 50 km altitude. The H₂O mixing ratio drops very rapidly above 70 km.

The comparison of the results from strong and weak H₂O and CO₂ lines shows the need to refine the line profile model.

INTRODUCTION

Infrared absorption spectrometry of the atmosphere, using the sun as a light source at sunrise or sunset, has for the past 15 years proved to be a powerful method of studying vertical distributions of trace species. The largest possible amount of light-absorbing molecules is observed on the optical path tangent to the earth's surface at various altitudes, allowing the deconvolution of very low concentrations as a function of altitude. A great deal of information has already been gathered with this method from high-altitude platforms such as aircraft and balloons. An orbiting platform provides access to higher altitudes and to nearly global coverage. Whereas with high-altitude platforms the earth's rotation provides altitude scanning at sunrise or sunset, scanning is achieved at a much higher rate from an orbiting spacecraft. Such fast spectral scanning requires a high-throughput instrument.

One of the main goals of the grille spectrometer operating on the Spacelab pallet was to observe trace species in the low thermosphere and in the mesosphere such as CO₂, CO, H₂O and CH₄. Preliminary data on this later molecule have already been published [1]. A part of the results on the three others will be presented here. They confirm previous mass spectrometric measurements on CO₂ in the transition atmospheric region, the turbopause, where mixing is replaced by diffusion. They show the large increase of the CO mixing ratio at altitudes where the CO₂ photodissociation by the solar H Lyman α radiation takes place and where the H₂O abundance vanishes abruptly.

INSTRUMENTATION

The optics consists of a two-axis steerable frontal plane mirror which tracks the sun in front of a Cassegrain telescope with aperture 30 cm and focal length 6 m. The sun is imaged on the grille, which intercepts a square portion of the solar image (8 arc minutes). The spectrometer has a grating of 58 grooves per millimeter, which is illuminated by a parabolic mirror oscillating at 436 Hz with an amplitude of ± 20 arc seconds; the position of the mirror is controlled within 2 arc seconds. The exit light flux, split into two beams, passes through interference filters to two detectors (InSb, 2.5 to 5.5 μm , and HgCdTe, 2.5 to 10.5 μm). The spectral resolving power is at least 1.3×10^4 (instrumental line width at half peak height). Using data originating from the orbiter (time, attitude, and orbit parameters) and from Spacelab (timeline, onboard and ground commands, sun ephemeris), its processors manage the execution of the stored measurement programs, including in flight updating. The electronics on the pallet instrument provides the functions of electromechanical control and signal detection and formatting. The flight crew performed a wavelength alignment 12 hours after launch.

TREATMENT OF THE DATA

Narrow spectral intervals of the central part of the solar disk are rapidly scanned while the sun is rising or setting. Telluric absorption features are then analysed using the onion peeling method on the basis of the absorption lines parameters /2/ adapted for the atmospheric temperature and pressure conditions of the Mid Latitude - Spring Fall model. A Voigt line shape is used. The observed equivalent widths are inverted by successive iteration every 2 km from high to low altitudes.

The results presented below are very sensitive to the Spacelab orbital data; the solar angle attributed to each observation is derived from NASA preliminary orbital data available immediately after the flight. An improved version (Post Flight Altitude and Trajectory History) should be available in the near future. The observed spectra are also generated from recordings made during and immediately after the flight operations. An improved data set should soon be distributed to the experimenters. It may lead to modify the results presented here below.

RESULTS

Carbon dioxide

Several portions of absorption runs were scheduled during the mission to observe CO_2 at the highest possible altitudes where its mixing ratio has been already shown to depart from its homospheric values (3,4). The region of the strongest absorption lines was chosen (near 4.24 μm). Measurements for two runs are shown in Fig. 1. Event 13 has been studied in detail and the results from two lines are shown as obtained in the linear part of their curve of growth where the equivalent width is small but very reliable since the line width is practically only due to Doppler broadening. The line parameters are reproduced in Table 1.

Up to 100 km altitude, using non saturated lines, the CO_2 volume mixing ratio follows closely the 3×10^{-4} value and drops abruptly above by a factor of 10 over 15 kilometers. These findings are in good agreement with the mass spectrometric data (3,4). These results give great confidence in the data used from the instrument.

Carbon monoxide

It is known that carbon dioxide must be most strongly photodissociated in the upper mesosphere and thermosphere by solar U.V. radiation /5/. Few ground based mesospheric CO measurements have been published /6,7/, all show a large mixing ratio increase from the stratopause to the mesopause.

Two absorption runs provided data on CO during the Spacelab One Mission. The spectral lines used are listed in Table 1 and the inverted abundances are shown in figure 2. The P_6 line was observed at sunset in the northern hemisphere yielding equivalent widths at 70 km which are at the upper limit of low linear part of the curve of growth leading to some uncertainty on the maximum value observed at that altitude. In addition this line is contaminated by O_3 absorptions below 60 km precluding CO determinations at lower altitude. The other observation took place at sunrise in the southern hemisphere. In this case the weaker R_2 line was used which provided data down to the low stratosphere where a mixing ratio value equal to 10^{-8} is reached at 30 km altitude in agreement with balloon borne measurements /8,9/.

In both cases the thermospheric upper values are in good agreement indicating (figure 1) an equal abundance of CO and CO₂ at 115 ± 5 km altitude. At lower altitudes the vertical profiles exhibit similar shapes with a maximum abundance near the production peak. Figure 2 also shows a well marked change in the CO profile at the turbopause level which occurs at higher altitude in the northern hemisphere observation than in the southern hemisphere run. The results indicate also a large variability of the mesospheric CO.

The simulation of CO solar lines is achieved in agreement with Rinsland et al /10/ using the Minnaert formula /11/ instead of the Beer Lambert law. The linestrengths are those calculated by Seals /12/ at 4500 K, and the value of the saturation constant Rc was chosen at 33% of absorption. The solar line shape is very close to the one calculated by Muller and Sauval /13/. The spectra computed with this simulation are in good agreement with the solar spectra recorded during the Spacelab 1 Mission in the spectral ranges : (2154-2163), (2118-2124), (2206-2210) cm⁻¹.

Table 1.- Line parameters used : integrated absorption cross section at 296°K, (S), in cm; energy of the upper state (E) in cm⁻¹; pressure half width₁ at half peak height, (W_p), in cm⁻¹ and at one atmosphere; wavenumber, (ν), in cm⁻¹.

Species		S	E	W _p
CO ₂	2357.835	7.77 x 10 ⁻²⁰	1031.129	.069
	2358.728	3.53 x 10 ⁻¹⁸	60.871	.074
CO	2119.681	3.65 x 10 ⁻¹⁹	80.735	.072
	2154.596	2.60 x 10 ⁻¹⁹	11.535	.080
	2158.300	3.29 x 10 ⁻¹⁹	23.070	.077
	2161.969	3.82 x 10 ⁻¹⁸	39.448	.075
H ₂ O	3816.092	2.10 x 10 ⁻¹⁹	79.496	.094
	3819.905	9.30 x 10 ⁻²¹	136.762	.094
	3824.281	3.47 x 10 ⁻²²	142.274	.092
	3818.341	9.16 x 10 ⁻²²	709.606	.082

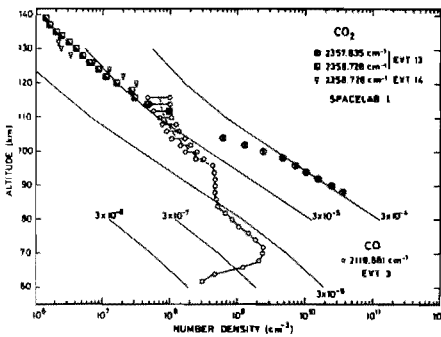


Fig. 1. Number density of CO₂ and CO in molecules per cm³ versus altitude using two different CO₂ absorption lines and the P₆ CO line. The nearly parallel lines represent constant volume mixing ratios from 3 x 10⁻⁸ to 3 x 10⁻⁴.

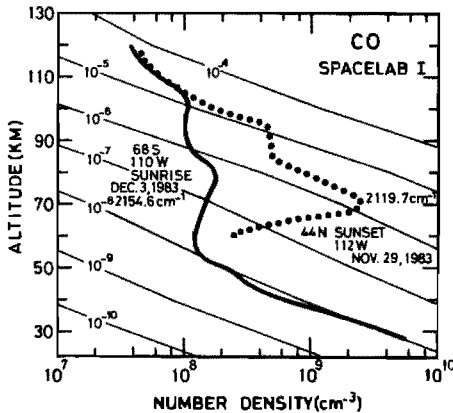


Fig. 2. Carbon monoxide number density versus altitude retrieved from two solar occultation runs, one in the southern hemisphere at sunrise and the other one in the northern hemisphere at sunset. The geographic coordinates of the solar rays tangent points at 50 km altitude are indicated. Two different absorption lines were used of which the wavenumbers are indicated. The nearly parallel lines represent constant volume mixing ratios from 10⁻¹⁰ to 10⁻⁴. The dates of data capture are also given.

Water vapor

Water vapor abundance in the stratosphere and the mesosphere have been recently measured using spectrometric techniques : in the microwave region from the ground /14,15/ and with a rocket borne radiometer in the 2.7 μm region /15/; they indicate a wide range of mixing ratio values : from 1 to 15 parts per million in volume depending of altitude and techniques. Several of our Spacelab runs were dedicated to the measurement of this trace constituent so important for the middle atmosphere aeronomy. Two wavelength regions were selected : 6.3 and 2.7 μm . Due to a better signal to noise ratio at the short wavelength, the results of a sample run near 3820 cm^{-1} are shown here.

Figure 3 shows the retrieved abundance of H_2O versus altitude for the linear part of the curve of growth for 4 lines. The data has been also analysed in the region where the lines saturate and all agree on a mixing ratio close to 3 ppm at 30 km, at higher altitudes especially around 60 km, there is disagreement between lines of different strengths. This could be resolved by studying the absorption line profile which in these cases drives the equivalent width even more than the H_2O concentration. Work currently in progress on this subject could help solve similar difficulties encountered on the interpretation of H_2O data from other infrared instruments /16,17/.

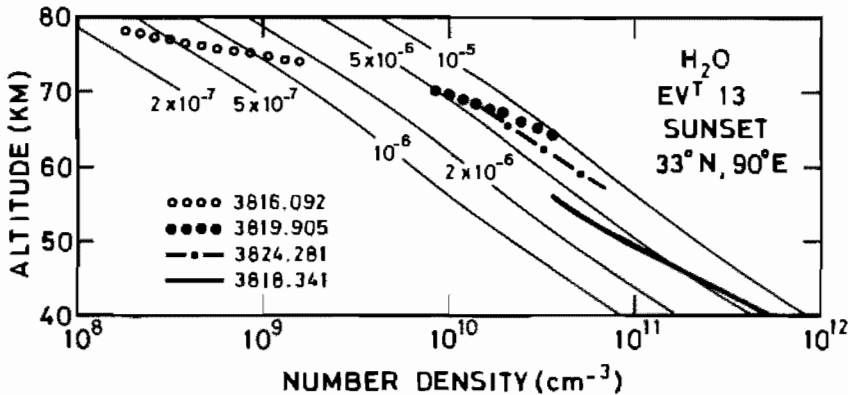


Fig. 3. Water vapor number densities versus altitude retrieved using only lines in the regions where their curve of growth is quasi linear. The nearly parallel lines represent constant volume mixing ratios from 10^{-7} to 10^{-5} .

At the present time of the retrieval process, the following features can be assessed on the water vapor mixing ratio abundance versus the altitude : a tendency to increase from 30 to 50 km and a decrease by a factor of at least 20 occurs from 72 to 80 km.

DISCUSSION AND CONCLUSION

Vertical distributions of carbon monoxide in the mesosphere and in the thermosphere combined with distributions of carbon dioxide show for the first time where these two species present equal abundances. They also show CO variability indicating the need for more measurements. The water vapor vertical distribution in the middle atmosphere exhibit, for the case studied, a small variation with altitude up to about 70 km where the volume concentration drops abruptly. More observations performed during the mission will allow to refine this picture.

Previous observations from rockets and satellites have already indicated the need to depart from the standard convolution of a Doppler and Lorentz profile. This paper confirms this result, the higher resolution of our spectra permits us to use lines which are close to the linear region of the curve of growth for H_2O and CO_2 . To reconcile these results to what we obtain from the more intense lines, we need a more complete investigation of the atmospheric absorption processes, which in turn, would affect the models used to compute atmospheric cooling rates /18/.

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